Supporting Information

Factors Dictating Carbene Formation at (PNP)Ir.

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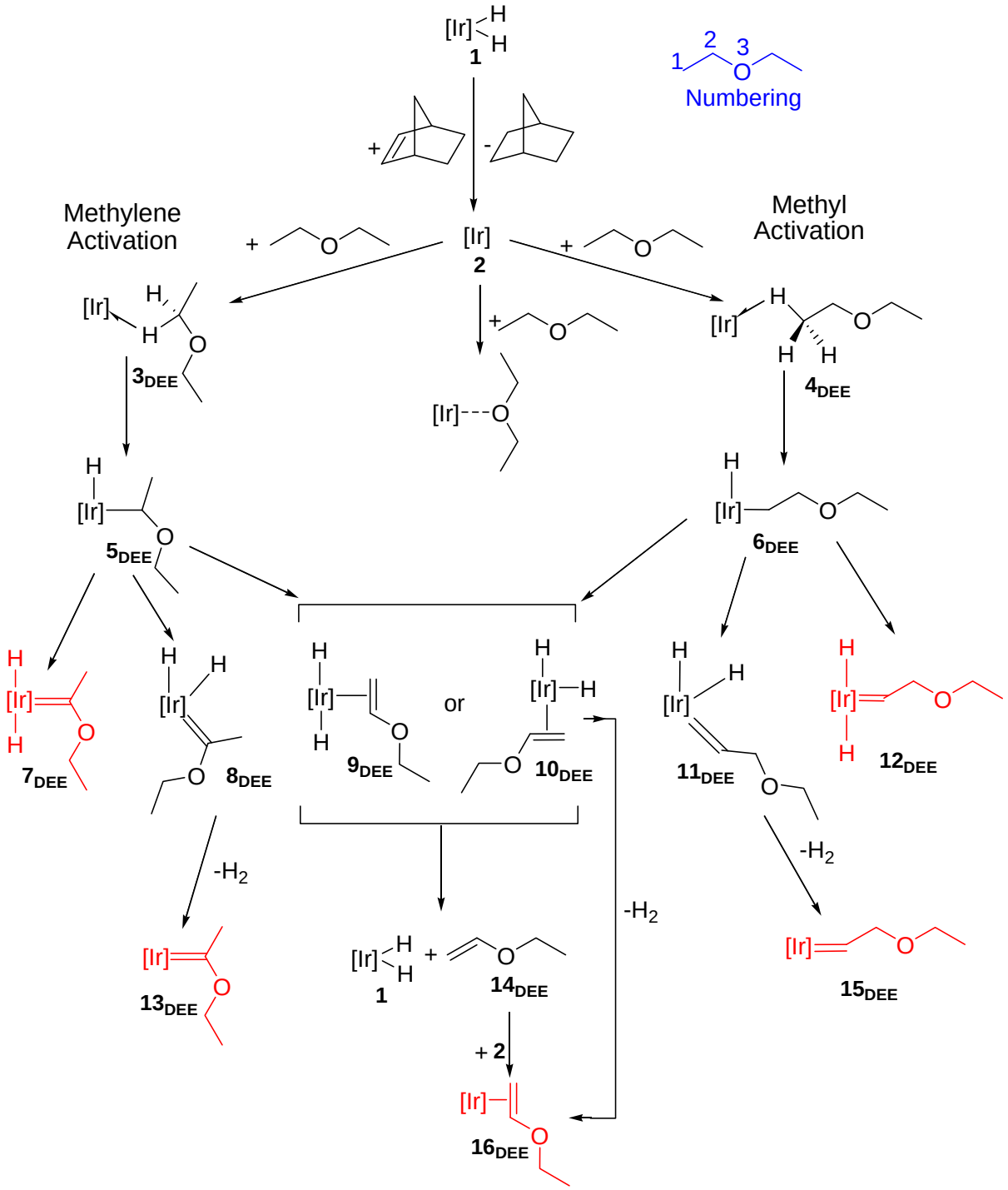
1. Diethyl Ether (DEE)

1.1. Experimental reaction of (PNP)IrH$_2$ (1) with Norbornylene in Diethyl Ether

(PNP)IrH$_2$ (**1**) and norbornylene (3 equiv) were combined in DEE (700 µL), and the resulting brown solution was transferred to a J. Young tube. ^{31}P NMR spectroscopy after 10 min revealed generation of 2 intermediate species (δ 47.5 and 29.5 ppm, in a 2:3 ratio). The solution was frozen and the headspace evacuated and backfilled with carbon monoxide (1 atm). As the solution thawed, an immediate color change from brown to yellow was observed, and ^{31}P NMR spectroscopy revealed a mixture containing 2 new species (δ 28.9 and 27.3 ppm, in a 3:2 ratio) as the major products, along with small amounts of (PNP)Ir–CO (δ 57.6 ppm) and *cis*-(PNP)Ir(H)$_2$(CO) (δ 47.4 ppm), each comprising approximately 6% of the total mixture. Volatiles were removed from this mixture in vacuo and the residues redissolved in C_6D_6 to allow ^{1}H NMR characterization. ^{1}H NMR spectroscopy revealed hydride signals at δ –7.81 (t, $^2J_{PH}$ = 18 Hz) and –8.12 (t, $^2J_{PH}$ = 18 Hz) in a 3:2 ratio, consistent with previous reports for (PNP)Ir(H)(R)(CO) species.[1,2]

1.2. Diethyl ether relative energy diagrams

Scheme S1



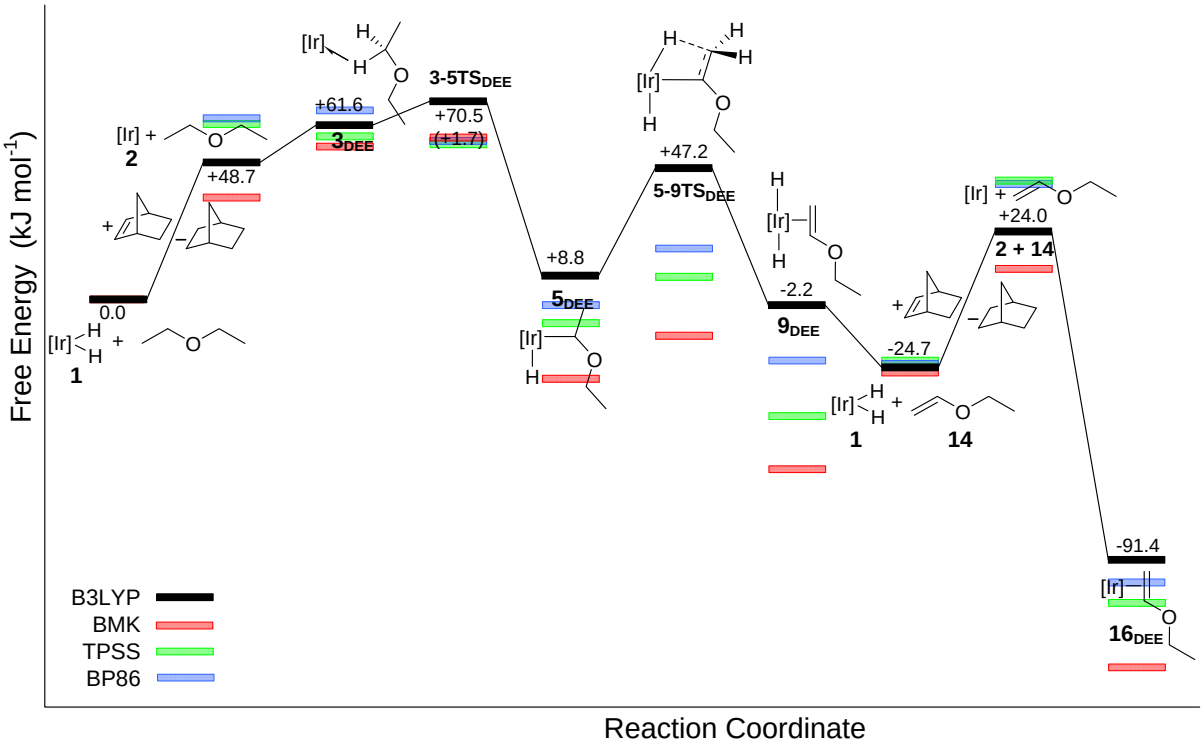


Figure S1. Relative energy surface for the formation of vinyl ether **16**$_{DEE}$ via C2 coordination. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

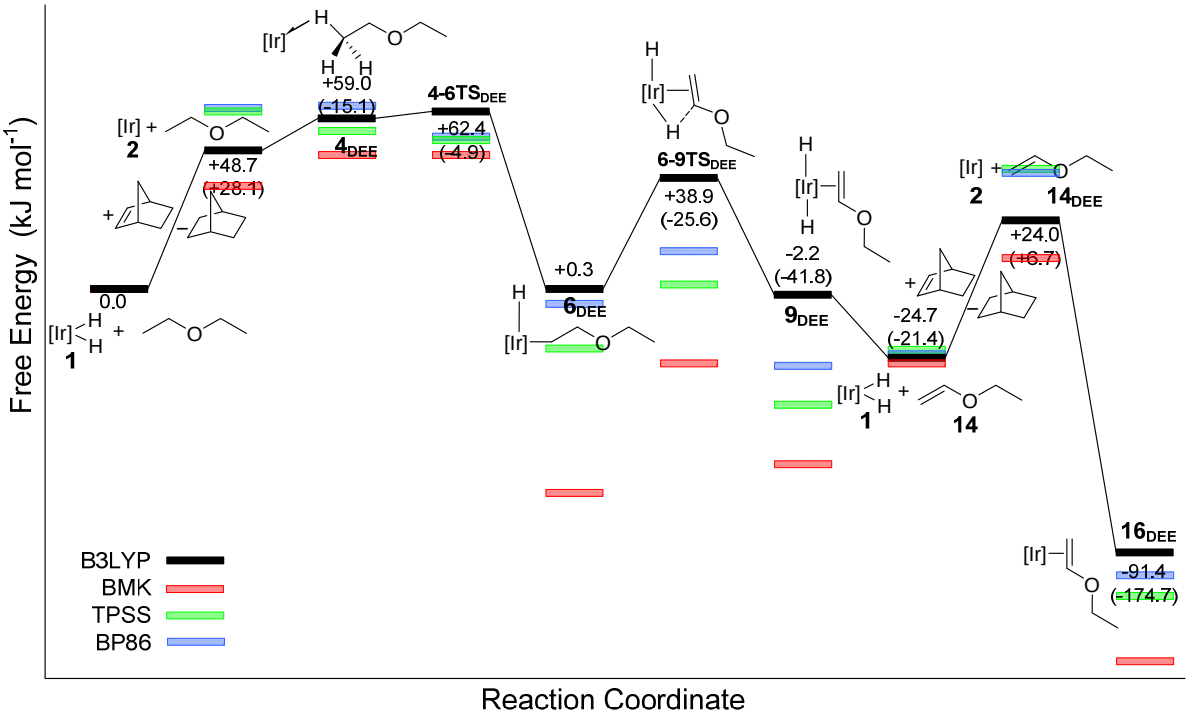


Figure S2. Relative energy surface for the formation of vinyl ether **16**$_{DEE}$ via C1 coordination. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

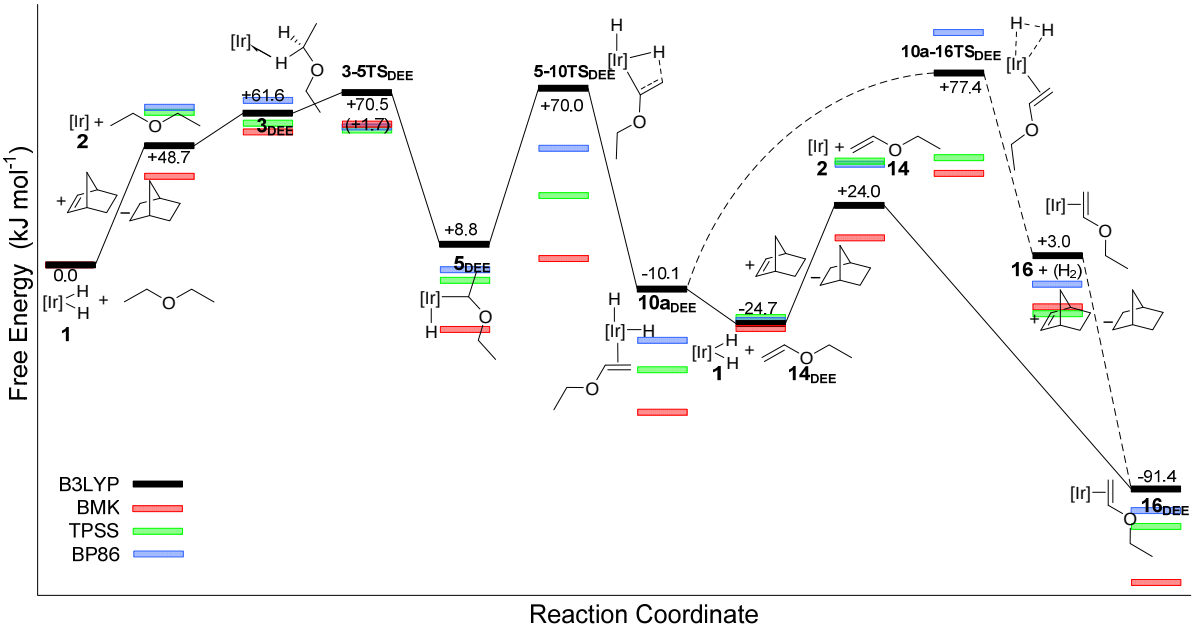


Figure S3. Relative energy surface for the formation of vinyl ether **16**$_{DEE}$ via C2 coordination and cis oxidative addition. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

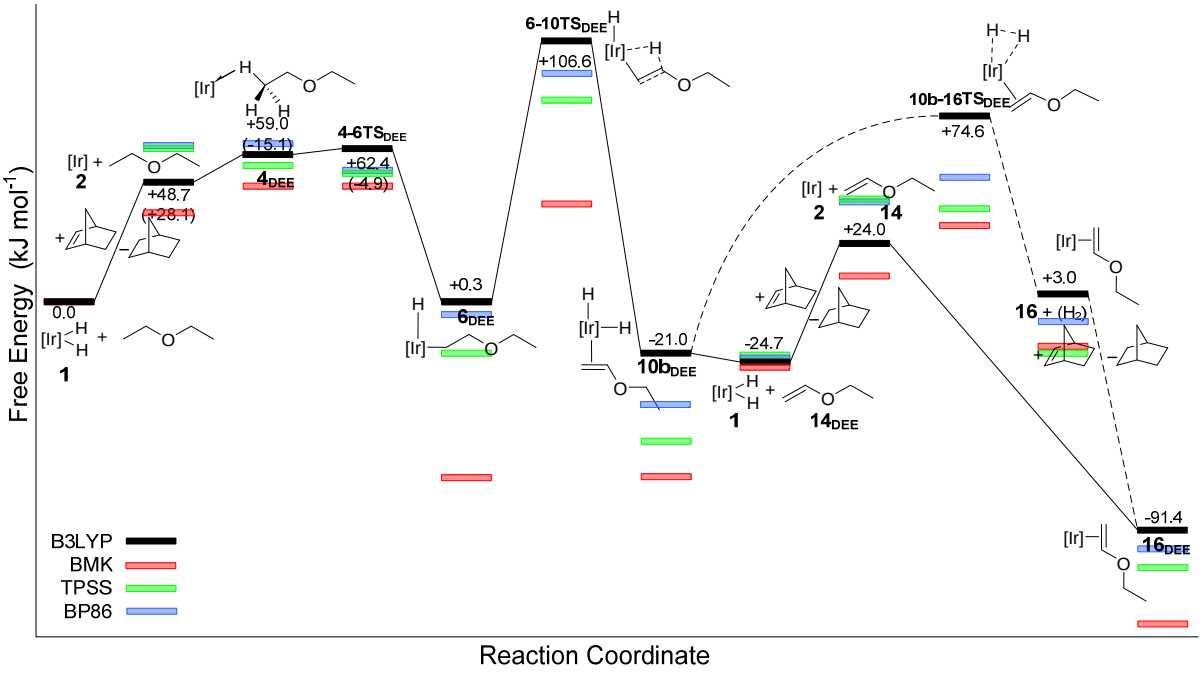


Figure S4. Relative energy surface for the formation of vinyl ether **16**$_{DEE}$ via C1 coordination and cis oxidative addition. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

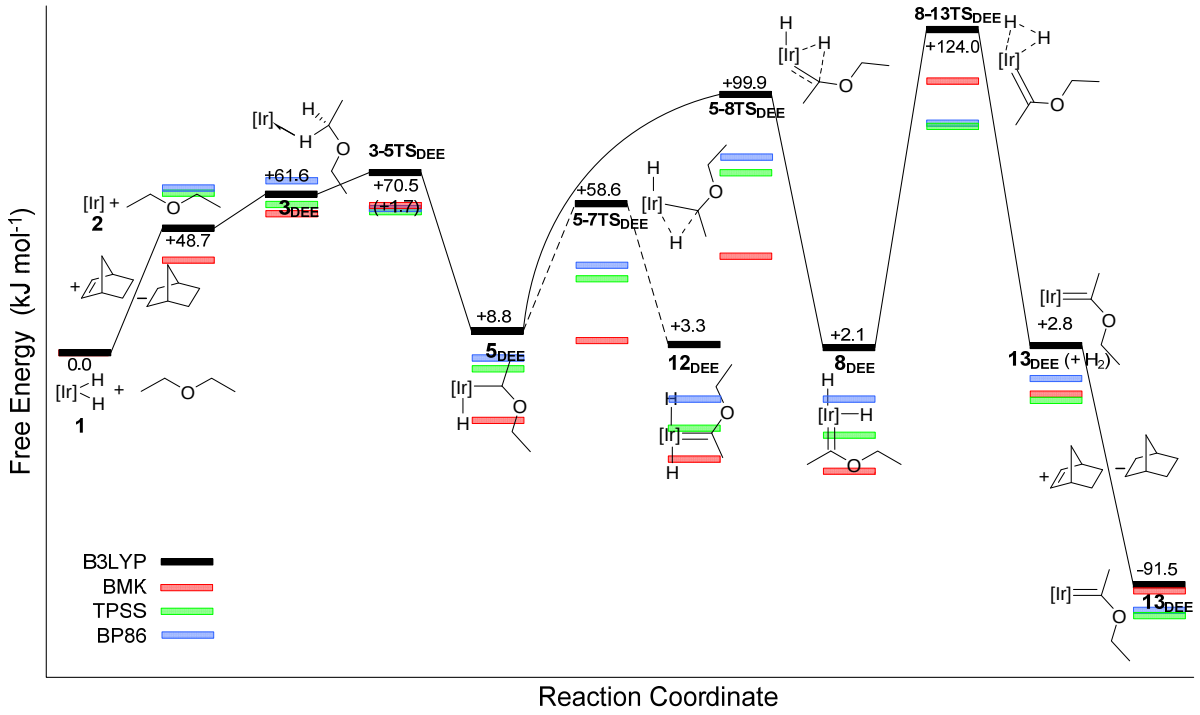


Figure S5. Relative energy surface for the formation of carbene **13**$_{DEE}$ via C2 coordination. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

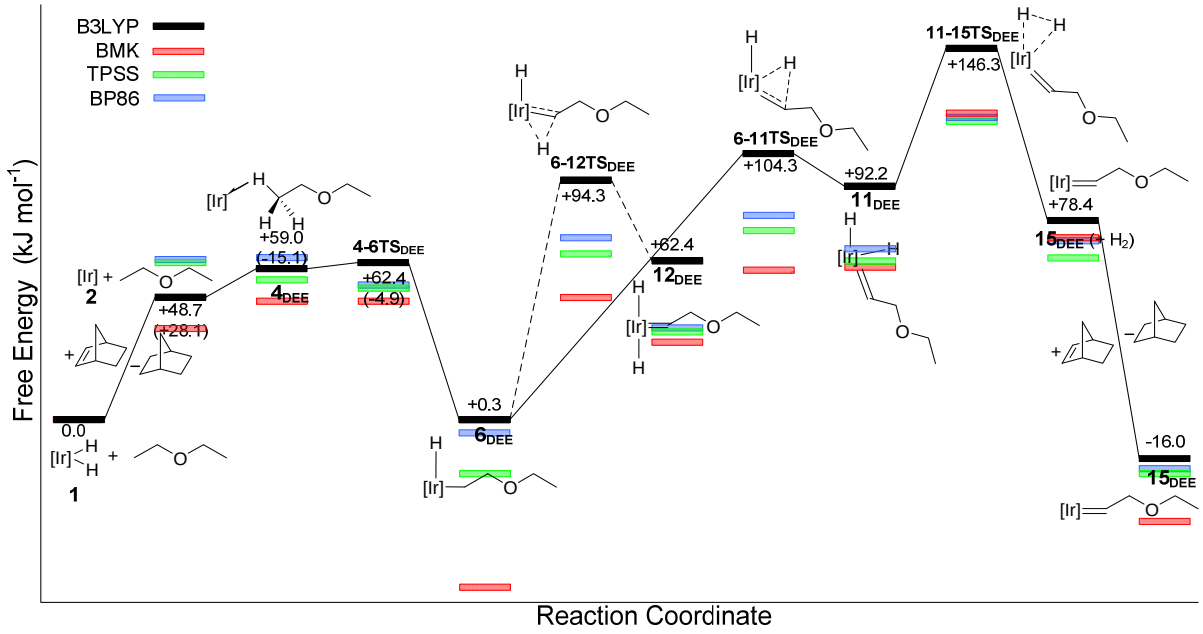


Figure S6. Relative energy surface for the formation of carbene **13**$_{DEE}$ via C1 coordination. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

1.3. Alternate reactions of DEE with (PNP)IrH$_2$ (1)

We noted in Scheme 2 that alternate pathways are available that provide the same final product **16**$_{DEE}$. One other such pathway that is equally likely to provide **16**$_{DEE}$ is via initial coordination at the C2 position followed by the second oxidative addition from C1. This is displayed in Figure S7 where the reaction coordinates for **9**$_{DEE}$ through **16**$_{DEE}$ are identical to those already discussed.

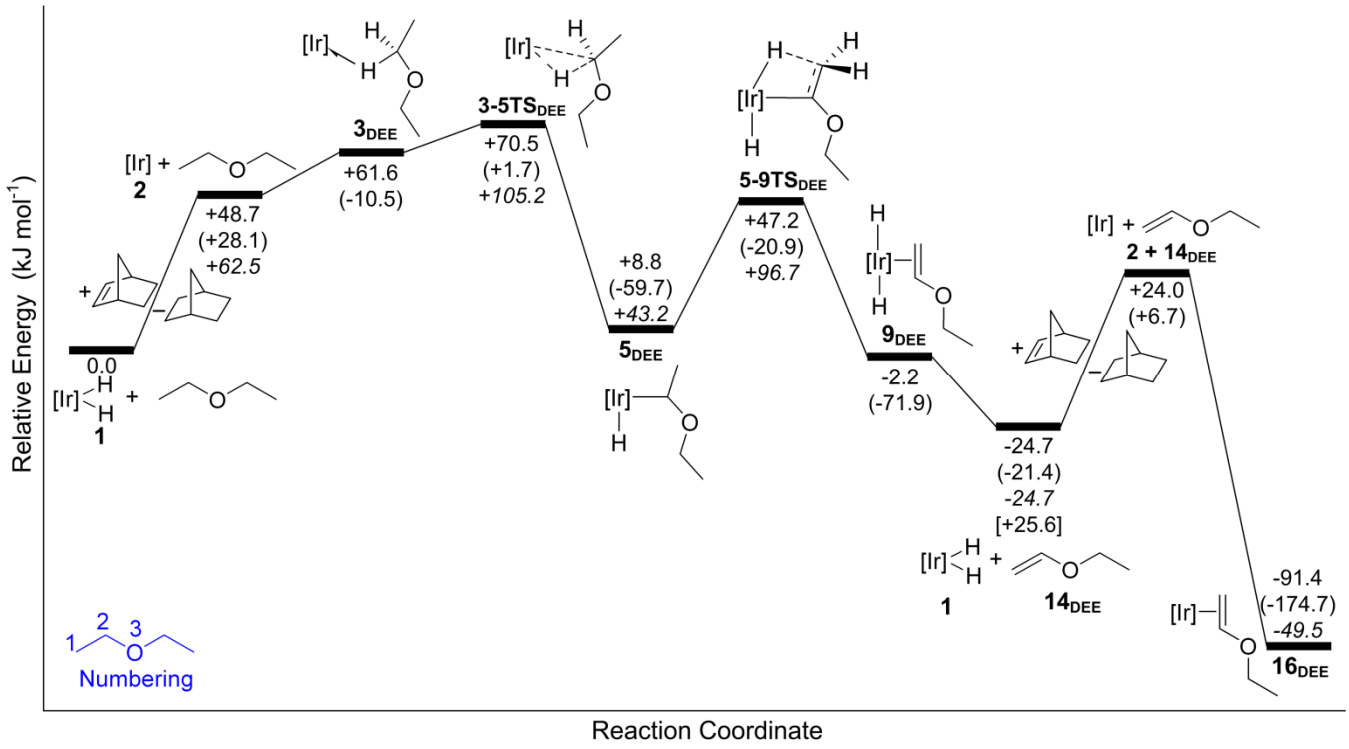


Figure S7. Relative energy surface for the formation of vinyl ether **16**$_{DEE}$ via C2 initial coordination. Values in normal script and parentheses are Model-opt Gibbs corrected and uncorrected electronic energies respectively. Values in italics and square brackets are Full-opt and MP2/GBS2 energies respectively, both Gibbs corrected. All values in kJ mol^{-1}.

If we compare Figure S7 to Figure 1 in the main text we find that both relative energy surfaces are remarkably similar and so it would appear that two equally likely pathways to **16**$_{DEE}$ exist. The methylene C-H activation pathway in Figure S7 shows some less favorable conditions such as the higher barrier to initial C-H activation at **3-5TS**$_{DEE}$ (+70.5 versus +62.4 kJ mol^{-1}), a marginally less stable intermediate **5**$_{DEE}$ (+8.8 versus +0.3 kJ mol^{-1}) and a slightly

higher transition barrier at **5-9TS$_{DEE}$** (+47.2 versus +38.9 kJ mol^{-1}). But in general, both methylene and methyl C-H activation paths could coexist.

Given the potential for two coexisting pathways we would predict that two intermediates **5$_{DEE}$** and **6$_{DEE}$** would be observed in the slowly reacting mixture. The experimental findings in this regard match exactly this prediction. First, it has been previously reported that two intermediate species were observed to form during the preparation of **16$_{DEE}$**, with both of these proceeding to the same vinyl ether adduct.[2] Second, these intermediate species have been trapped as six-coordinate CO adducts, in a manner previously reported for *tert*-butyl methyl ether (TBE) and 1,4-dioxane (DIO) substrates, and spectroscopic data suggest that the trapped products are both carbonyl adducts of iridium(III) alkyl hydrides. Although definitive assignment of these adducts has thus far not been possible, their existence provides strong support that the two intermediates present are from single C-H activation steps. Our theory suggests these to be the C2 methylene C-H and C1 methyl C-H activated structures **5$_{DEE}$** and **6$_{DEE}$**, and the fact that they are formed experimentally in similar quantities (ca. 60:40 ratio) supports a small energy difference between the two pathways.

There are other pathways which lead to the formation of **16$_{DEE}$**. Scheme 2 indicates these to be centered around initial formation of **10$_{DEE}$** (from either **5$_{DEE}$** or **6$_{DEE}$**) which in turn leads to either vinyl ether or dihydrogen elimination. These pathways (some of which are displayed in section 1.1 are plausible but require higher activation energies, and given the lower energy alternatives already outlined in Figures 1 (manuscript) and S7, these pathway are unlikely to contribute.

As yet the competing carbene formation reaction as seen in many of the other linear ether reactions with **1**, has not been considered. Figure S8 outlines the relative energy surface for one such carbene formation pathway, in fact the lowest energy carbene pathway for the DEE + **1** reaction. It should be noted this pathway is not observed experimentally.

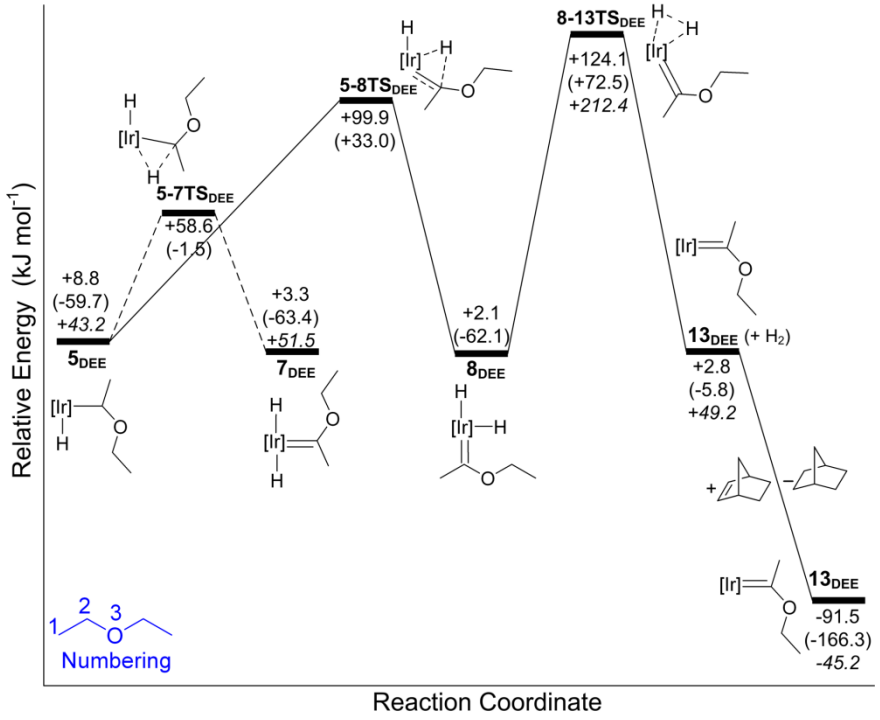


Figure S8. Relative energy surface for the formation of carbene **13**$_{DEE}$ from intermediate **5**$_{DEE}$. Values in normal script and parentheses are Model-opt Gibbs corrected and uncorrected electronic energies respectively. Values in italics are Full-opt energies. All values in kJ mol^{-1}.

We start from the familiar intermediate **5**$_{DEE}$ in Figure S8, which is one likely structure present after the initial methylene hydrogen elimination. As found previously,[1,3] the second α-hydrogen migration has two possible directions, one being to the trans-dihydrido structure **7**$_{DEE}$ and the other its cis equivalent **8**$_{DEE}$. The path to **8**$_{DEE}$ faces a significant barrier at **5-8TS**$_{DEE}$ of +99.9 kJ mol^{-1}, but it is the subsequent reaction step that becomes a critical

point in this reaction pathway. It has a barrier at **8-13TS$_{DEE}$** of +124.1 kJ mol^{-1} at the Model-opt level of theory prior to forming the carbene **13$_{DEE}$** + H_2, which goes some way to explain the experimental absence of the thermodynamically stable carbene **13$_{DEE}$** (which is even more stable once the hydrogen is reacted indirectly[3] with excess norbornylene).

The pathway to the trans-dihydro carbene **7$_{DEE}$** shown in Figure S8 has little impact on the reaction since no subsequent reaction coordinates exist, but we will show that the dihydro carbene will become an important reaction coordinate for other ether reactions. For this reason it becomes relevant to note that thermodynamically this structure is of similar energy to **5$_{DEE}$**, **9$_{DEE}$** and higher in energy than **1** + **14$_{DEE}$**.

1.4. Carbene position from DEE reactions with (PNP)IrH$_2$ (1)

Alkoxycarbene formation always occurs at the carbon adjacent to the etheral oxygen and the structures discussed throughout this chapter show the same trend. But given the array of differing reaction paths available in the DEE sequence it seems pertinent to discuss the factors responsible for this preference.[4]

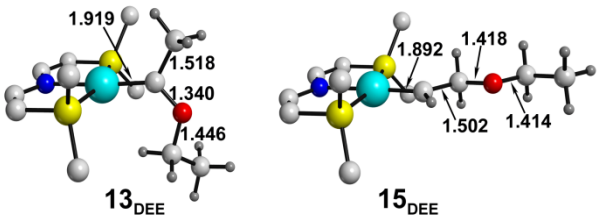


Figure S9. Model-opt geometries of diethyl ether carbenes at the C2 (**13$_{DEE}$**) and C1 (**15$_{DEE}$**) positions. All measurements in Å. Hydrogens are omitted from the [Ir] fragment.

Consider Figure S9 which has displayed two possible carbenes **13$_{DEE}$** and **15$_{DEE}$**, with the C2 carbene **13$_{DEE}$** being significantly more stable than the C1 analogue **15$_{DEE}$** (-91.5 versus -16.0 kJ mol^{-1} respectively – see Figure S8 and others in section 1.1 above). But notice from the figure that the more stable **13$_{DEE}$** has a longer/weaker Ir-$C_{carbene}$ bond than **15$_{DEE}$** (1.919 versus 1.892 Å respectively) and also a shorter/stronger $C_{carbene}$-O bond. Electron population analysis also reveals that the ether fragment of **13$_{DEE}$** has an NBO positive charge of +0.225 compared to the neutral (+0.003) ether fragment on **15$_{DEE}$**. The charge transferred from the ether fragment in **13$_{DEE}$** is retained on the iridium metal centre which now has an NBO charge of -0.612 (cf. -0.417 for **15$_{DEE}$**).

This apparent imbalance in electron distribution and difference in energetic stability between the two structures is caused by the electron deficiency of the Fischer carbene. The metal is not solely able to compensate for the electron deficient carbene and so π donation from the electron rich oxygen atom occurs. The diagram below in Figure S10, taken from the book by Crabtree, outlines the arrangement.[5] The competing donation from atoms adjacent to the $C_{carbene}$ is perhaps best illustrated by the resonance structures II and III, with structure III closely resembling the real arrangement for **13$_{DEE}$**. This creates a negatively charged metal, a strong O-$C_{carbene}$ bond and ultimately an energetically stable species.

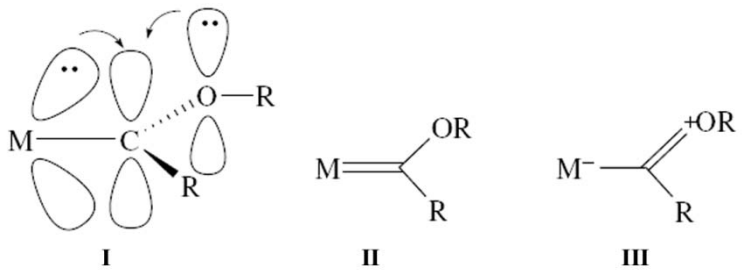


Figure S10. Fischer carbene structures in the presence of lone pairs from oxygen. Taken from the book by Crabtree.[5]

This concept applies to all of the carbene (or potential carbenes in the DEE case) involving ether substrates. Carbenes will only form at the carbon directly adjacent to the oxygen.

1.5. Preferred Orientation for Vinyl Ether and Carbene

Figure S11 depicts the ideal orientation for both vinyl ether and carbene. Note the ideal carbene has the O-C-R ether and the (PNP)Ir framework coplanar, thus allowing for greater metal back donation, while the ideal vinyl ether O-C-C orientation is orthogonal to the (PNP)Ir plane.[6]

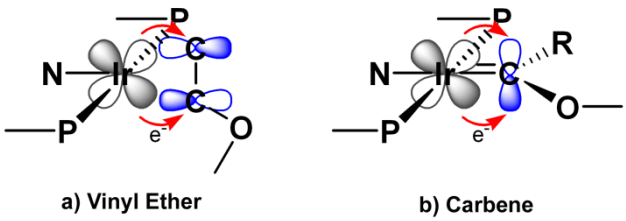


Figure S11. a) Preferred vinyl ether orientation with the O-C-C ether fragment orthogonal to the (PNP)Ir plane, b) Preferred carbene orientation with the O-C-R ether fragment coplanar with the (PNP)Ir framework.

1.6. Coordinates of DEE structures at the Model-opt level of Theory

Diethyl Ether
B3LYP/GBS(1) = -233.659386 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -233.742014 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -233.572076 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -233.770500 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -233.728311 a.u
M06/GBS(2)//B3LYP/GBS(1) = -233.5613493 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -233.070627 a.u.
Enthalpy Correction = 0.145264
Gibbs Free Energy Correction = 0.107422

Atomic No	x-coord	y-coord	z-coord
6	-2.378807	-0.416733	0.000028
6	-1.182294	0.521811	-0.000160

1	-3.314216	0.153795	-0.001105
1	-2.361846	-1.059458	-0.886254
1	-2.363013	-1.057872	0.887476
1	-1.206101	1.178790	-0.887457
1	-1.206198	1.179308	0.886750
6	1.182299	0.521786	0.000152
1	1.206083	1.179161	-0.886855
1	1.206275	1.178899	0.887346
6	2.378801	-0.416726	-0.000123
1	2.362357	-1.058538	-0.887057
1	3.314185	0.153799	-0.000168
1	2.362575	-1.058761	0.886653
8	-0.000011	-0.256244	0.000161

Norbornane

B3LYP/GBS(1) = -273.963973 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -274.046026a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -273.847900 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -274.092664a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -274.032915 a.u.
M06/GBS(2)//B3LYP/GBS(1) = 273.8186086 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -272.9661801 a.u.
Enthalpy Correction = 0.184582
Gibbs Free Energy Correction = 0.149043

Atomic No	x-coord	y-coord	z-coord
6	-1.255680	-0.782709	-0.493750
6	0.000011	-1.133596	0.340249
6	-0.000010	1.133596	0.340249
6	-1.255702	0.782686	-0.493737
1	-1.208925	-1.206174	-1.503414
1	-2.161351	-1.177057	-0.018444
1	-1.208983	1.206172	-1.503393
1	-2.161372	1.177000	-0.018401
6	-0.000002	0.000000	1.389182
1	0.891277	0.000008	2.028350
1	-0.891283	-0.000009	2.028348
6	1.255702	-0.782689	-0.493735
1	2.161375	-1.176999	-0.018402
1	1.208983	-1.206169	-1.503393
6	1.255680	0.782711	-0.493747
1	2.161353	1.177055	-0.018442
1	1.208928	1.206175	-1.503412
1	0.000017	-2.155722	0.731168
1	-0.000020	2.155723	0.731166

Norbornylene

B3LYP/GBS(1) = -272.722693 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -272.805319 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -272.611798 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -272.855129 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -272.7952478 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -272.580379 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -271.7589184a.u.
Enthalpy Correction = 0.159859
Gibbs Free Energy Correction = 0.125197

Atomic No	x-coord	y-coord	z-coord
6	1.191072	0.781215	-0.516488
6	-0.088270	1.128551	0.322933
6	-0.087690	-1.128566	0.323018
6	1.191573	-0.780702	-0.516270
1	1.146187	1.206946	-1.523336
1	2.088508	1.178211	-0.027995
1	1.147098	-1.206730	-1.523010
1	2.089177	-1.177017	-0.027528
6	-0.041153	0.000052	1.380753
1	-0.912375	-0.000148	2.043397
1	0.878469	0.000315	1.979534
6	-1.279351	0.670027	-0.507648
1	-1.921211	1.328259	-1.085475
6	-1.278851	-0.670674	-0.507820
1	-1.920234	-1.329254	-1.085780
1	-0.120316	2.157640	0.689572
1	-0.119286	-2.157637	0.689750

Structure 1
B3LYP/GBS(1) = -1157.898649a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1158.11644a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1157.0636295 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1158.14678051 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1158.24206196 a.u.
Enthalpy Correction = 0.261248
Gibbs Free Energy Correction = 0.199716

Atomic No	x-coord	y-coord	z-coord
7	-0.000031	1.638003	-0.000224
6	-1.203018	2.307354	0.000140
6	-2.400183	1.663281	0.000295
1	-1.156235	3.400176	0.000281
1	-3.334112	2.217345	0.000371
6	1.202978	2.307329	0.000209
6	2.400129	1.663251	0.000361
1	1.156221	3.400152	0.000375
1	3.334058	2.217321	0.000497
15	-2.305480	-0.141519	0.000126
15	2.305532	-0.141566	0.000178
6	-3.312480	-0.724116	-1.437636
1	-3.340456	-1.818448	-1.446718
1	-4.337087	-0.338767	-1.385262
1	-2.845295	-0.380527	-2.364246
6	-3.311164	-0.724583	1.438601
1	-4.335905	-0.339469	1.387303
1	-3.338846	-1.818931	1.447330
1	-2.843188	-0.381231	2.364900
6	3.312261	-0.724052	-1.437830
1	4.336750	-0.338334	-1.385869
1	3.340621	-1.818378	-1.446734
1	2.844637	-0.380794	-2.364340
6	3.311669	-0.724507	1.438372
1	3.339547	-1.818851	1.447070
1	4.336328	-0.339214	1.386763
1	2.843925	-0.381252	2.364824
77	-0.000032	-0.454062	-0.000317

1	0.000120	-1.800885	-0.850197
1	-0.000327	-1.800600	0.850012

Structure 2
B3LYP/GBS(1) = -1156.658443a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1156.865021a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1155.821627a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1156.893255a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1156.98712149 a.u.
Enthalpy Correction = 0.244383
Gibbs Free Energy Correction = 0.18372

Atomic No	x-coord	y-coord	z-coord
7	1.386923	1.601318	-0.089570
6	2.754828	1.495233	-0.137330
6	3.406748	0.303219	-0.106026
1	3.294758	2.441034	-0.202999
1	4.490263	0.254224	-0.145585
6	0.786574	2.835505	-0.124199
6	-0.561042	3.005011	-0.079588
1	1.468183	3.684828	-0.190730
1	-1.004059	3.995390	-0.108954
15	2.323946	-1.120527	0.003455
15	-1.488059	1.475124	0.028628
6	2.888957	-2.115278	1.463313
1	2.301862	-3.037237	1.539333
1	3.949788	-2.378851	1.378201
1	2.734957	-1.529456	2.373283
6	2.780015	-2.251975	-1.393589
1	3.845202	-2.510054	-1.364499
1	2.192228	-3.174857	-1.336517
1	2.555279	-1.755089	-2.340981
6	-2.607719	1.627219	1.499409
1	-3.242314	2.518229	1.425457
1	-3.249809	0.742686	1.575421
1	-1.998258	1.692842	2.404498
6	-2.720356	1.493655	-1.357415
1	-3.363541	0.608536	-1.299684
1	-3.350064	2.390280	-1.317369
1	-2.184235	1.471956	-2.309802
77	0.267231	-0.044205	0.031515

Structure 3 (oxygen bound ether)
B3LYP/GBS(1) = -1390.348411a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.632349a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.42462996 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.696552 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.744520 a.u.
Enthalpy Correction = 0.391981
Gibbs Free Energy Correction = 0.31527

Atomic	No	x-coord	y-coord	z-coord
7		-0.069574	-2.143937	-0.013682
6		1.087371	-2.872340	-0.029120
6		2.317751	-2.290382	-0.038194

1	0.973477	-3.958484	-0.033096
1	3.226710	-2.883882	-0.049011
6	-1.271201	-2.798998	0.004387
6	-2.464614	-2.144217	0.026800
1	-1.223564	-3.890111	0.000187
1	-3.406054	-2.684684	0.039334
15	2.280753	-0.500619	-0.020430
15	-2.317936	-0.360289	0.027533
8	-0.020907	2.154892	0.004475
6	3.366276	0.041874	-1.432961
1	3.502045	1.129723	-1.421493
1	4.353906	-0.430991	-1.372404
1	2.894642	-0.242135	-2.377671
6	3.357863	0.008965	1.411052
1	4.341745	-0.471774	1.352057
1	3.503604	1.095491	1.421244
1	2.873450	-0.288021	2.345263
6	-3.382191	0.244893	-1.372645
1	-4.402620	-0.146955	-1.286131
1	-3.427001	1.339633	-1.373666
1	-2.952839	-0.089076	-2.320974
6	-3.322207	0.247817	1.469644
1	-3.358674	1.343086	1.473639
1	-4.348349	-0.136015	1.423614
1	-2.856664	-0.090709	2.399061
77	-0.011735	-0.109361	-0.007026
6	0.548836	2.777334	1.175591
6	-0.131730	2.282328	2.436738
1	0.418202	3.862892	1.066083
1	1.625593	2.561334	1.197628
1	0.317783	2.778376	3.305502
1	-1.200661	2.516555	2.419751
1	-0.011573	1.198269	2.532285
6	0.452391	2.775892	-1.210528
6	-0.373740	2.322369	-2.397854
1	1.510933	2.517075	-1.345065
1	0.376844	3.863753	-1.076145
1	0.035034	2.765201	-3.313881
1	-0.343364	1.230144	-2.474435
1	-1.415824	2.640952	-2.294723

Structure 3-DEE

B3LYP/GBS(1) = -1390.333068 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.621733 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.406624 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.68521622 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.734953 a.u.
Enthalpy Correction = 0.390504
Gibbs Free Energy Correction = 0.310745

Atomic No	x-coord	y-coord	z-coord
7	1.400668	1.703427	-0.490494
6	0.859027	2.957336	-0.608590
6	-0.442899	3.228942	-0.323599
1	1.541092	3.739752	-0.947389
1	-0.845295	4.231854	-0.425609
6	2.726830	1.502533	-0.770196
6	3.331478	0.290270	-0.645087

1	3.281710	2.381949	-1.103414
1	4.384868	0.158199	-0.871019
15	-1.382572	1.804976	0.224137
15	2.243613	-1.010609	-0.067202
8	-2.433906	-2.112429	0.022880
6	-2.899478	1.711744	-0.840305
1	-3.530970	0.881341	-0.506440
1	-3.478014	2.641810	-0.792104
1	-2.599876	1.529583	-1.875987
6	-2.139620	2.246559	1.859468
1	-2.730581	3.167404	1.789113
1	-2.792473	1.435094	2.199793
1	-1.342926	2.385542	2.594917
6	2.404767	-2.417191	-1.268890
1	3.447180	-2.743277	-1.364291
1	1.800832	-3.270165	-0.937593
1	2.040893	-2.092138	-2.247249
6	3.045576	-1.748154	1.435971
1	2.465553	-2.606298	1.793816
1	4.067035	-2.081689	1.217970
1	3.075316	-0.994262	2.227019
77	0.249207	0.158978	0.136671
6	-1.316720	-2.084630	0.856504
6	-1.720474	-2.487863	2.268332
1	-0.928929	-1.004847	0.994661
1	-0.512548	-2.722815	0.475205
1	-0.863530	-2.410964	2.944655
1	-2.517571	-1.835628	2.638534
1	-2.087973	-3.519301	2.270956
6	-2.116298	-2.095955	-1.370102
6	-3.412549	-2.097807	-2.161563
1	-1.511877	-2.985095	-1.614641
1	-1.499449	-1.207099	-1.583784
1	-3.196413	-2.111733	-3.235603
1	-4.016069	-2.978941	-1.918373
1	-4.005817	-1.204317	-1.942102

Structure 3-5TS - DEE

B3LYP/GBS(1) = -1390.324123 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.617105 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.4038451 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.684987 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.7378413 a.u.
Enthalpy Correction = 0.386396
Gibbs Free Energy Correction = 0.309494
Imaginary Freq = -711.0i

Atomic No	x-coord	y-coord	z-coord
7	1.512949	1.700406	-0.566947
6	2.865785	1.538377	-0.710430
6	3.497986	0.359990	-0.458807
1	3.427747	2.417790	-1.035549
1	4.571593	0.257039	-0.582214
6	0.950862	2.944239	-0.705991
6	-0.362060	3.187710	-0.453668
1	1.622166	3.746403	-1.023062
1	-0.784846	4.180491	-0.573732
15	2.420932	-0.954095	0.119655

15	-1.301032	1.753449	0.088473
8	-2.147775	-1.671578	-0.539556
6	3.071047	-1.489015	1.770674
1	2.505095	-2.351465	2.139303
1	4.131319	-1.760458	1.709564
1	2.949530	-0.665205	2.478539
6	2.807827	-2.443622	-0.917892
1	3.874467	-2.692748	-0.874525
1	2.232808	-3.308551	-0.567727
1	2.532017	-2.237976	-1.955992
6	-1.981589	2.152083	1.766074
1	-2.551728	3.088152	1.752156
1	-2.636881	1.341238	2.102129
1	-1.151678	2.244415	2.471180
6	-2.856929	1.759255	-0.917035
1	-3.500473	0.935211	-0.595211
1	-3.394302	2.706799	-0.793617
1	-2.613891	1.625387	-1.974532
77	0.343077	0.103215	0.037787
6	-0.904570	-1.860645	0.086411
6	-1.133314	-2.802579	1.276202
1	-0.530227	-0.823605	1.046485
1	-0.197188	-2.334063	-0.602157
1	-0.197356	-2.976314	1.818084
1	-1.860963	-2.380303	1.977965
1	-1.523370	-3.762474	0.917827
6	-2.092038	-1.554159	-1.959517
6	-3.508452	-1.632325	-2.506860
1	-1.484308	-2.377099	-2.369791
1	-1.597243	-0.614183	-2.237743
1	-3.493880	-1.567119	-3.600813
1	-3.979759	-2.578794	-2.221656
1	-4.126878	-0.814646	-2.123646

Structure 4 - DEE

B3LYP/GBS(1) = -1390.334173 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.623484 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.410643 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.685677 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.736442 a.u.
Enthalpy Correction = 0.390786
Gibbs Free Energy Correction = 0.311482

Atomic No	x-coord	y-coord	z-coord
7	-0.337686	-2.203190	0.260081
6	0.887684	-2.748082	-0.032145
6	1.912558	-2.020657	-0.549548
1	0.996234	-3.813747	0.179630
1	2.872298	-2.476955	-0.771129
6	-1.320481	-2.989177	0.800092
6	-2.550875	-2.510253	1.130414
1	-1.060041	-4.038154	0.955330
1	-3.313090	-3.154748	1.556659

15	1.520604	-0.289675	-0.813851
15	-2.764740	-0.765165	0.793143
8	0.719825	3.317318	-1.441041
6	1.917548	0.094370	-2.582601
1	1.708043	1.151291	-2.773845
1	2.969038	-0.115273	-2.812519
1	1.280928	-0.516490	-3.228691
6	2.808648	0.700453	0.076552
1	3.817459	0.459032	-0.279057
1	2.612391	1.764869	-0.083867
1	2.743435	0.485655	1.146631
6	-4.295649	-0.604781	-0.246640
1	-5.161222	-1.066845	0.242745
1	-4.520906	0.452071	-0.430310
1	-4.123481	-1.095690	-1.208226
6	-3.337553	0.025657	2.372328
1	-3.556673	1.086629	2.206140
1	-4.239997	-0.462333	2.759227
1	-2.540080	-0.052099	3.116002
77	-0.678548	-0.238319	-0.081372
6	-0.573176	3.517657	-0.902787
6	-1.301028	2.186053	-0.745575
1	-1.161390	4.165076	-1.576014
1	-0.504451	4.037793	0.067750
1	-2.332143	2.368133	-0.433963
1	-1.302299	1.628153	-1.685797
1	-0.781544	1.645716	0.126211
6	1.410994	4.540570	-1.655382
6	2.763457	4.250526	-2.284961
1	1.535104	5.073553	-0.697613
1	0.814095	5.193848	-2.314297
1	3.303478	5.186806	-2.464376
1	3.373887	3.621781	-1.628983
1	2.641863	3.733605	-3.242463

Structure 4-6TS - DEE

B3LYP/GBS(1) = -1390.326798 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.619609 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.406967 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.685422 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.73832581 a.u.
Enthalpy Correction = 0.386559
Gibbs Free Energy Correction = 0.308905
Imaginary Freq = -720.1i

Atomic No	x-coord	y-coord	z-coord
7	1.811402	1.603921	0.002963
6	1.324573	2.888483	0.030838
6	-0.003288	3.171769	-0.012231
1	2.069689	3.685350	0.096294
1	-0.361102	4.196611	0.010742
6	3.157680	1.373179	0.110921
6	3.690415	0.121350	0.145861

1	3.796978	2.257462	0.173124
1	4.761231	-0.035278	0.230465
15	-1.076486	1.729320	-0.104839
15	2.480810	-1.200334	0.039534
8	-3.152752	-1.153601	-0.417994
6	-2.191123	1.989373	-1.559687
1	-2.864268	1.131535	-1.645219
1	-2.778902	2.908910	-1.455125
1	-1.581582	2.056700	-2.465366
6	-2.255226	1.851581	1.315130
1	-2.824367	2.787996	1.282760
1	-2.943906	1.003303	1.275898
1	-1.688706	1.806037	2.249052
6	3.025506	-2.307392	-1.347120
1	4.045697	-2.675086	-1.187031
1	2.352126	-3.168024	-1.431280
1	2.990569	-1.746051	-2.284798
6	2.752648	-2.303356	1.504498
1	2.089874	-3.173928	1.447876
1	3.790769	-2.652241	1.553013
1	2.517130	-1.745643	2.414619
77	0.503368	0.018507	-0.121459
6	-2.193165	-2.198010	-0.401619
6	-0.817732	-1.691097	-0.841863
1	-2.510723	-2.992080	-1.100784
1	-2.151315	-2.652670	0.603521
1	-0.173878	-2.567519	-0.947619
1	-0.925566	-1.209306	-1.819169
1	-0.496443	-1.141873	0.451187
6	-4.460494	-1.617372	-0.118410
6	-5.445735	-0.466147	-0.242199
1	-4.486288	-2.041593	0.899762
1	-4.735597	-2.429647	-0.812861
1	-6.462170	-0.815126	-0.028427
1	-5.203801	0.336354	0.462139
1	-5.429631	-0.051298	-1.255465

Structure 5 - DEE

B3LYP/GBS(1) = -1390.350693 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.640468 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.436272 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.708499 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.759759 a.u.
Enthalpy Correction = 0.387473
Gibbs Free Energy Correction = 0.309384

Atomic No	x-coord	y-coord	z-coord
7	1.357242	1.798526	0.200355
6	2.727199	1.719777	0.197319
6	3.395560	0.546828	0.024125
1	3.275632	2.656845	0.334240
1	4.480935	0.513369	0.029953
6	0.708161	3.009377	0.245470
6	-0.641927	3.122195	0.132028
1	1.333509	3.898588	0.370909
1	-1.127609	4.092371	0.180661

15	2.358115	-0.906045	-0.230655
15	-1.541322	1.569599	-0.078607
8	-2.219431	-1.682290	0.530488
6	2.949260	-2.185871	0.972608
1	2.391959	-3.118206	0.830431
1	4.017832	-2.388277	0.837552
1	2.781826	-1.832306	1.993819
6	2.869417	-1.655783	-1.843580
1	3.945387	-1.863013	-1.861241
1	2.321874	-2.590003	-2.006192
1	2.622434	-0.962786	-2.651979
6	-2.843782	1.545194	1.233610
1	-3.542930	2.380121	1.110200
1	-3.379235	0.593634	1.179765
1	-2.368376	1.622909	2.215399
6	-2.553339	1.738074	-1.616632
1	-3.189718	0.854838	-1.732020
1	-3.185510	2.632399	-1.579210
1	-1.885180	1.803381	-2.479189
77	0.222572	0.030831	-0.082764
6	-0.814824	-1.609843	0.778394
6	-0.655313	-1.464320	2.291363
1	-0.355116	-0.839273	-1.267891
1	-0.369786	-2.564030	0.456960
1	0.400703	-1.485330	2.577966
1	-1.086095	-0.523224	2.650235
1	-1.168460	-2.286934	2.810572
6	-2.584064	-2.297245	-0.685912
6	-4.100513	-2.419021	-0.740874
1	-2.118679	-3.295411	-0.759067
1	-2.208039	-1.705424	-1.537577
1	-4.411273	-2.906868	-1.671849
1	-4.472268	-3.010609	0.102406
1	-4.574022	-1.431620	-0.696989

Structure 5-7TS -DEE

B3LYP/GBS(1) = -1390.322652 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.618328 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.421367 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.692608 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.742432 a.u.
Enthalpy Correction = 0.381922
Gibbs Free Energy Correction = 0.306192
Imaginary Freq = -826.1i

Atomic No	x-coord	y-coord	z-coord
7	1.432819	1.795280	-0.398090
6	0.828127	3.010912	-0.430930
6	-0.508362	3.171800	-0.215441
1	1.466705	3.876710	-0.632294
1	-0.972856	4.152054	-0.266182
6	2.781334	1.681279	-0.474053
6	3.426256	0.493571	-0.292790
1	3.347810	2.594699	-0.680924
1	4.506784	0.420130	-0.373331

15	-1.441505	1.676267	0.105132
15	2.396262	-0.926137	0.066721
8	-2.288107	-1.348015	0.060199
6	-2.772479	1.641509	-1.180199
1	-3.431730	0.787502	-1.010832
1	-3.359894	2.566681	-1.153663
1	-2.306057	1.541738	-2.163860
6	-2.422075	1.933371	1.650549
1	-3.060223	2.821350	1.573824
1	-3.048457	1.054192	1.831543
1	-1.732728	2.052980	2.489944
6	2.914630	-2.194011	-1.191371
1	4.008379	-2.258985	-1.223393
1	2.518855	-3.188813	-0.962049
1	2.548955	-1.885986	-2.174692
6	3.042141	-1.694017	1.623956
1	2.490154	-2.613304	1.848768
1	4.108914	-1.931640	1.539047
1	2.892015	-0.989676	2.445785
77	0.234115	0.042755	0.092334
6	-0.934679	-1.514926	-0.035779
6	-0.517172	-2.970113	-0.141189
1	0.620125	0.578615	1.576173
1	-0.401938	-0.826757	-1.378881
1	0.561086	-3.052709	-0.233380
1	-0.823437	-3.488898	0.777577
1	-0.973807	-3.496762	-0.987931
6	-3.216391	-2.350164	-0.398407
6	-4.619233	-1.871477	-0.064196
1	-3.019489	-3.308098	0.094861
1	-3.094814	-2.489770	-1.481420
1	-5.352588	-2.626217	-0.369377
1	-4.722157	-1.705642	1.013118
1	-4.855249	-0.936714	-0.581769

Structure 5-8TS - DEE

B3LYP/GBS(1) = -1390.306603 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.605177 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.411675 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.679314 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.729115 a.u.
Enthalpy Correction = 0.383456
Gibbs Free Energy Correction = 0.308769
Imaginary Freq = -128.4i

Atomic No	x-coord	y-coord	z-coord
7	1.260198	-1.732628	-0.589958
6	2.608654	-1.683805	-0.779752
6	3.352080	-0.579660	-0.506281
1	3.071067	-2.594108	-1.166426
1	4.423204	-0.561936	-0.681813
6	0.599715	-2.919271	-0.733142
6	-0.714920	-3.069475	-0.430659
1	1.194719	-3.754774	-1.107173
1	-1.224093	-4.016221	-0.582054

15	2.446887	0.821572	0.135254
15	-1.548418	-1.587481	0.130210
8	-2.239172	1.432695	-0.498975
6	3.079638	2.258214	-0.863677
1	2.819678	3.218217	-0.406289
1	4.172302	2.194568	-0.925473
1	2.665821	2.219351	-1.874736
6	3.153343	1.249826	1.794473
1	4.231631	1.436258	1.730502
1	2.661240	2.145548	2.189799
1	2.966419	0.418975	2.478504
6	-3.022763	-1.452248	-0.979002
1	-3.527889	-2.424306	-1.027822
1	-3.718447	-0.695451	-0.615920
1	-2.690146	-1.166765	-1.979792
6	-2.346415	-1.953494	1.758719
1	-2.915124	-1.079706	2.094780
1	-3.024599	-2.811310	1.683619
1	-1.566411	-2.167493	2.493253
77	0.253451	-0.074238	0.158757
6	-0.850021	1.545160	-0.398509
6	-0.371292	2.960640	-0.682986
1	0.743416	-0.828961	1.532964
1	-0.575698	1.339125	0.885677
1	0.708775	3.034842	-0.595725
1	-0.642525	3.213460	-1.716268
1	-0.812365	3.731686	-0.035029
6	-3.062559	2.486486	0.015520
6	-4.509456	2.018875	-0.007523
1	-2.956014	3.395423	-0.590789
1	-2.752899	2.730599	1.044345
1	-5.171379	2.822376	0.335190
1	-4.806451	1.738620	-1.023552
1	-4.655839	1.153180	0.647079

Structure 5-9TS - DEE

B3LYP/GBS(1) = -1390.326844 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.625715 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.430598 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.702808 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.751650 a.u.
Enthalpy Correction = 0.382744
Gibbs Free Energy Correction = 0.309237
Imaginary Freq = -832.8i

Atomic No	x-coord	y-coord	z-coord
7	1.298849	1.839300	-0.301723
6	2.634646	1.776301	-0.527700
6	3.333273	0.603368	-0.497075
1	3.144350	2.719846	-0.744350
1	4.403163	0.582063	-0.680983
6	0.608661	3.006922	-0.376333
6	-0.743536	3.073321	-0.210805

1	1.189075	3.910873	-0.583524
1	-1.269543	4.020928	-0.280029
15	2.375458	-0.872321	-0.164100
15	-1.588845	1.512428	0.051220
8	-2.214658	-1.831699	0.424417
6	3.204883	-1.755294	1.239365
1	2.717925	-2.718627	1.429230
1	4.261291	-1.939927	1.013495
1	3.138535	-1.139786	2.140915
6	2.670028	-2.058325	-1.552801
1	3.736567	-2.284527	-1.667248
1	2.126268	-2.991886	-1.370274
1	2.291607	-1.611090	-2.475022
6	-2.652174	1.691694	1.554438
1	-3.352259	2.527749	1.445751
1	-3.220106	0.768310	1.708685
1	-2.017371	1.871662	2.426577
6	-2.869202	1.391352	-1.276762
1	-3.500563	0.513315	-1.113373
1	-3.501664	2.286698	-1.286841
1	-2.366973	1.294001	-2.242253
77	0.227615	0.022227	0.107123
6	-0.825976	-1.759761	0.628269
6	-0.418240	-1.183496	1.896257
1	0.086446	-0.103885	-1.524080
1	-0.326466	-2.683538	0.322144
6	-2.563052	-2.278081	-0.877744
6	-4.068367	-2.488674	-0.932036
1	-2.041864	-3.224892	-1.097587
1	-2.227392	-1.542804	-1.623844
1	-4.368378	-2.836396	-1.926933
1	-4.381045	-3.234886	-0.194008
1	-4.604732	-1.557448	-0.718061
1	0.360175	0.194217	1.820522
1	-1.211401	-0.786713	2.525465
1	0.368466	-1.683785	2.454612

Structure 5-10TS - DEE

B3LYP/GBS(1) = -1390.315333 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.615592 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.42365 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.691213 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.740049 a.u.
Enthalpy Correction = 0.382611
Gibbs Free Energy Correction = 0.307798
Imaginary Freq = -530.2i

Atomic No	x-coord	y-coord	z-coord
7	-0.624365	-0.961063	1.526517
6	-1.784388	-0.679562	2.178733
6	-2.781381	0.071005	1.628931
1	-1.888679	-1.099300	3.182071
1	-3.695138	0.279525	2.176652
6	0.290689	-1.822112	2.058860
6	1.392484	-2.240247	1.380036
1	0.086250	-2.175210	3.072263

1	2.104599	-2.923730	1.832133
15	-2.481601	0.634497	-0.042021
15	1.548153	-1.626204	-0.297201
8	2.019693	1.692177	0.402789
6	-2.839337	2.454991	-0.070866
1	-2.734471	2.850921	-1.087716
1	-3.861392	2.651109	0.272780
1	-2.141919	2.981045	0.586332
6	-3.848586	0.003127	-1.115951
1	-4.829017	0.319445	-0.741171
1	-3.721091	0.373642	-2.139007
1	-3.795946	-1.087653	-1.133473
6	3.292049	-1.051151	-0.509256
1	3.991181	-1.842502	-0.215048
1	3.476016	-0.796638	-1.559321
1	3.444024	-0.161074	0.101565
6	1.530552	-3.098562	-1.419425
1	1.661177	-2.776493	-2.458431
1	2.331135	-3.802153	-1.162127
1	0.561327	-3.593591	-1.328922
77	-0.325807	-0.213692	-0.395109
6	0.699547	1.685267	-0.098076
1	0.099334	2.464323	0.379089
6	2.617956	2.982570	0.391711
6	3.989883	2.894153	1.042491
1	1.978907	3.695085	0.940261
1	2.702623	3.357737	-0.642849
1	4.465584	3.881106	1.069679
1	3.902166	2.521328	2.068237
1	4.642758	2.213696	0.485167
6	0.534437	1.566654	-1.557248
1	1.460557	1.458331	-2.122890
1	-0.178111	2.234403	-2.042868
1	-0.039841	0.396246	-1.999273
1	-1.111025	-1.563028	-0.963008

Structure 5-10bTS - DEE

B3LYP/GBS(1) = -1390.308817 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.604821 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.412282 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.67610739 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.725516 a.u.
Enthalpy Correction = 0.385853
Gibbs Free Energy Correction = 0.310988
Imaginary Freq = -206.7i

Atomic No	x-coord	y-coord	z-coord
7	-1.672206	1.589411	-0.012566
6	-1.204188	2.872405	0.047627
6	0.120250	3.180429	0.056543
1	-1.969561	3.648175	0.098123
1	0.452516	4.212332	0.112026
6	-3.011769	1.325747	0.008118
6	-3.518606	0.063977	-0.026583
1	-3.662187	2.199830	0.063086
1	-4.589781	-0.109901	-0.004795

15	1.230059	1.774667	0.008383
15	-2.297031	-1.242914	-0.086372
8	2.844321	-1.523951	0.465388
6	2.424595	1.962871	1.406516
1	3.113025	1.112005	1.408567
1	2.995110	2.894396	1.315706
1	1.873138	1.968345	2.350542
6	2.350212	1.968356	-1.451292
1	2.886975	2.923385	-1.417363
1	3.080789	1.152103	-1.460185
1	1.752541	1.918246	-2.364660
6	-2.719853	-2.432539	1.268810
1	-3.752060	-2.788178	1.170702
1	-2.046553	-3.296267	1.238696
1	-2.601856	-1.932132	2.233320
6	-2.646156	-2.277099	-1.583816
1	-1.956356	-3.127629	-1.623120
1	-3.673898	-2.658146	-1.572498
1	-2.496444	-1.663555	-2.475522
77	-0.345889	0.046996	-0.060178
6	1.463736	-1.826279	0.367160
1	1.297521	-2.917238	0.391223
6	3.624243	-2.105022	-0.568499
6	5.082529	-1.738267	-0.343480
1	3.278775	-1.742918	-1.552321
1	3.497878	-3.200872	-0.564070
1	5.712912	-2.183381	-1.121275
1	5.217666	-0.651592	-0.369396
1	5.423817	-2.101776	0.631198
6	0.662412	-1.101068	1.459885
1	1.350737	-0.560979	2.110441
1	0.086785	-1.804149	2.064375
1	1.137424	-1.538300	-0.683802
1	-0.584418	0.357878	-1.656511

Structure 6 - DEE

B3LYP/GBS(1) = -1390.355526 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.646502 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.455671 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.71678092 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.763446 a.u.
Enthalpy Correction = 0.387974
Gibbs Free Energy Correction = 0.312161

Atomic No	x-coord	y-coord	z-coord
7	1.131360	1.141574	-0.835070
6	0.585711	2.384694	-0.900372
6	-0.702146	2.641562	-0.521598
1	1.225146	3.192315	-1.271124
1	-1.112374	3.645373	-0.586566
6	2.436554	0.905346	-1.134597
6	3.014889	-0.322736	-0.977161
1	3.022983	1.749790	-1.510816

1	4.059250	-0.484259	-1.228120
15	-1.644556	1.242637	0.098704
15	1.959419	-1.609632	-0.301093
8	-1.016911	-1.690322	-1.974114
6	-3.268033	1.292391	-0.803594
1	-3.939533	0.512365	-0.428463
1	-3.754243	2.266103	-0.670741
1	-3.099796	1.129280	-1.871483
6	-2.204870	1.666123	1.812304
1	-2.766844	2.607043	1.826949
1	-2.840122	0.864490	2.204846
1	-1.326796	1.760414	2.456028
6	2.098437	-3.082537	-1.414281
1	3.146133	-3.358717	-1.578881
1	1.573410	-3.934915	-0.969771
1	1.628990	-2.849246	-2.372621
6	2.770815	-2.236060	1.239524
1	2.180568	-3.055483	1.663625
1	3.786838	-2.594395	1.037905
1	2.814485	-1.423557	1.969330
77	-0.077040	-0.490098	-0.103405
6	-1.945666	-2.338242	-1.051062
6	-1.310433	-2.162968	0.325635
1	-2.096184	-3.375030	-1.391673
1	-2.908266	-1.811638	-1.121267
1	-2.080684	-1.995555	1.086896
1	-0.753549	-3.060438	0.620479
1	0.360766	-0.104075	1.354546
6	-1.549274	-1.348693	-3.248237
6	-0.475133	-0.632926	-4.049406
1	-2.435024	-0.707035	-3.120663
1	-1.878356	-2.268842	-3.756097
1	-0.877084	-0.296371	-5.011668
1	-0.109750	0.236453	-3.492739
1	0.374423	-1.296065	-4.243245

Structure 6-9TS - DEE

B3LYP/GBS(1) = -1390.328941 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.627497 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.434348 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.703680 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.752204 a.u.
Enthalpy Correction = 0.38258
Gibbs Free Energy Correction = 0.307861
Imaginary Freq = -797.4i

Atomic No	x-coord	y-coord	z-coord
7	-1.010225	-1.457210	-1.201811
6	-2.262586	-1.275972	-1.693707
6	-3.075899	-0.258550	-1.284538
1	-2.607311	-1.996262	-2.441269
1	-4.072018	-0.134376	-1.698536
6	-0.265819	-2.545584	-1.533487

6	0.946412	-2.808455	-0.967020
1	-0.688864	-3.221368	-2.282323
1	1.522604	-3.682277	-1.256321
15	-2.408546	0.805324	-0.007638
15	1.502862	-1.640478	0.275674
8	2.260911	2.010357	0.199777
6	-3.585880	0.785307	1.419231
1	-3.234169	1.465711	2.202733
1	-4.594023	1.086864	1.112137
1	-3.616654	-0.227352	1.828112
6	-2.607309	2.551695	-0.602395
1	-3.651688	2.759732	-0.862162
1	-2.296907	3.261402	0.173133
1	-1.986924	2.701362	-1.490670
6	1.841073	-2.591437	1.826157
1	2.564455	-3.396222	1.651115
1	2.237183	-1.919064	2.595067
1	0.901559	-3.016564	2.186930
6	3.217923	-1.133429	-0.206680
1	3.620035	-0.420556	0.519045
1	3.878488	-2.006515	-0.262540
1	3.182538	-0.651123	-1.186937
77	-0.278608	-0.119718	0.291508
6	0.915674	1.903644	0.447338
6	0.519378	1.284500	1.697323
1	0.481266	1.028190	-0.795396
1	0.333632	2.758769	0.096831
6	2.603648	2.476548	-1.104518
6	4.106226	2.691509	-1.162739
1	2.066458	3.414903	-1.312776
1	2.272702	1.733331	-1.845997
1	4.395599	3.052901	-2.155585
1	4.421449	3.430517	-0.419115
1	4.640314	1.756487	-0.966655
1	-0.980058	-1.135098	1.360641
1	-0.225976	1.823910	2.279224
1	1.341652	0.917281	2.309354

Structure 6-11TS - DEE

B3LYP/GBS(1) = -1390.299530 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.600825 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.400206 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.674592 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.725069 a.u.
Enthalpy Correction = 0.382404
Gibbs Free Energy Correction = 0.306091
Imaginary Freq = -624.2

Atomic No	x-coord	y-coord	z-coord
7	-2.223708	0.676769	-0.629685
6	-2.432145	2.013330	-0.803894
6	-1.500273	2.948773	-0.480443
1	-3.400069	2.303342	-1.219353
1	-1.686539	4.006609	-0.639348
6	-3.214524	-0.224446	-0.882633

6	-3.088098	-1.555756	-0.625040
1	-4.136737	0.177739	-1.308729
1	-3.893553	-2.250091	-0.842831
15	0.043002	2.324353	0.186887
15	-1.533909	-2.051519	0.111296
8	3.624765	-0.980820	-0.163335
6	0.307963	3.126856	1.832646
1	1.276185	2.822874	2.244933
1	0.282734	4.219447	1.749083
1	-0.479456	2.793923	2.512534
6	1.354358	3.162275	-0.824698
1	1.145202	4.236526	-0.888668
1	2.344847	3.027528	-0.378527
1	1.358701	2.740809	-1.833486
6	-1.900869	-2.881766	1.721648
1	-2.588294	-3.724407	1.584757
1	-0.971807	-3.248273	2.171188
1	-2.350524	-2.150302	2.397034
6	-0.875936	-3.463448	-0.887523
1	0.042330	-3.855400	-0.437071
1	-1.612054	-4.273342	-0.941159
1	-0.650979	-3.112871	-1.897900
77	-0.408379	0.003992	0.177228
6	2.629440	-0.148820	-0.751509
6	1.264789	-0.734659	-0.569920
1	2.802761	-0.082827	-1.844791
1	2.706262	0.870550	-0.352353
1	1.375771	-1.823985	-0.618511
6	4.944220	-0.521447	-0.392249
6	5.914993	-1.486192	0.270710
1	5.072959	0.496246	0.017172
1	5.142443	-0.457808	-1.477092
1	6.949272	-1.160251	0.112993
1	5.726870	-1.538789	1.348059
1	5.799631	-2.492125	-0.146056
1	0.921019	-0.527755	1.060777
1	-1.223878	0.303666	1.579927

Structure 6-12TS - DEE

B3LYP/GBS(1) = -1390.304337 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.603323 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.402202 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.676452 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.726863 a.u.
Enthalpy Correction = 0.381774
Gibbs Free Energy Correction = 0.30479
Imaginary Freq = -757.9i

Atomic No	x-coord	y-coord	z-coord
77	0.412896	0.002285	0.186330
7	2.188367	0.773095	-0.773619
6	2.295124	2.107134	-1.000144
6	1.318530	2.988870	-0.645717

1	3.212867	2.456949	-1.482049
1	1.423115	4.051477	-0.844619
6	3.191867	-0.090131	-1.070636
6	3.135561	-1.421053	-0.770913
1	4.073174	0.328099	-1.566021
1	3.955008	-2.087825	-1.021306
15	-0.146262	2.303744	0.132472
15	1.662960	-1.975490	0.082051
6	-1.293214	-0.856098	0.357898
1	-1.374090	-1.946190	0.267033
6	-1.558169	2.992127	-0.856858
1	-2.517860	2.826456	-0.356713
1	-1.423260	4.070956	-0.996643
1	-1.580297	2.507182	-1.836436
6	-0.375380	3.192126	1.740260
1	-0.400147	4.278040	1.592729
1	-1.310736	2.876847	2.215319
1	0.454906	2.934591	2.402081
6	0.990838	-3.427025	-0.847650
1	1.745497	-4.216254	-0.939618
1	0.116538	-3.839260	-0.331801
1	0.687223	-3.100807	-1.845648
6	2.188343	-2.765636	1.669451
1	1.314969	-3.168901	2.193223
1	2.903084	-3.577271	1.490711
1	2.653319	-2.004967	2.301106
1	1.330052	0.405786	1.486641
1	-0.538841	-0.421595	-1.222835
6	-2.675577	-0.299074	0.493399
1	-2.733789	0.753646	0.189436
1	-2.909815	-0.334733	1.577690
8	-3.609483	-1.085402	-0.227587
6	-4.950544	-0.666872	-0.044020
1	-5.068348	0.385251	-0.356996
1	-5.220267	-0.716881	1.025845
6	-5.855627	-1.570036	-0.866410
1	-5.748932	-2.612273	-0.548308
1	-6.903887	-1.274736	-0.745801
1	-5.596186	-1.507796	-1.928205

Structure 7 - DEE

B3LYP/GBS(1) = -1390.347660 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.641895 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.441675 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.717075 a.u.
Enthalpy Correction = 0.38302
Gibbs Free Energy Correction = 0.308695

Atomic No	x-coord	y-coord	z-coord
7	-0.434622	-2.158611	-0.560522
6	-1.714953	-2.546472	-0.784823
6	-2.777707	-1.712533	-0.594861
1	-1.868996	-3.573018	-1.130205

1	-3.795836	-2.039477	-0.781843
6	0.603107	-3.012880	-0.740354
6	1.898210	-2.650961	-0.510801
1	0.360359	-4.023289	-1.082305
1	2.717527	-3.346756	-0.662489
15	-2.380953	-0.067568	-0.018003
15	2.147202	-0.968986	0.041200
8	0.609130	2.774074	0.235479
6	-3.358750	0.230390	1.524330
1	-3.202894	1.255398	1.879312
1	-4.430155	0.078638	1.348423
1	-3.013314	-0.464938	2.292998
6	-3.174420	1.130378	-1.185451
1	-4.250178	0.939383	-1.275762
1	-3.028151	2.157419	-0.832471
1	-2.703092	1.022186	-2.165233
6	3.113707	-1.029158	1.617754
1	4.056197	-1.573386	1.486327
1	3.337573	-0.011862	1.958682
1	2.505837	-1.527533	2.376497
6	3.381607	-0.200745	-1.106232
1	3.639810	0.809317	-0.768594
1	4.298743	-0.799590	-1.153088
1	2.938879	-0.139834	-2.103404
77	-0.044524	-0.141846	0.126265
6	0.299162	1.639385	0.847246
6	0.253696	1.947208	2.331565
1	0.060681	0.332200	-1.483086
1	-0.168179	-0.695078	1.717410
1	-0.703227	1.611490	2.741056
1	1.019981	1.351185	2.838224
1	0.408168	3.011524	2.540619
6	0.741674	2.888542	-1.203734
6	1.083267	4.338222	-1.499223
1	-0.196526	2.572100	-1.662557
1	1.518523	2.198283	-1.536554
1	1.195845	4.475244	-2.580399
1	0.292974	5.010133	-1.148317
1	2.021768	4.630111	-1.016257

Structure 8 - DEE

B3LYP/GBS(1) = -1390.347570 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.641387 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.441891 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.716650 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.764715
Enthalpy Correction = 0.384553
Gibbs Free Energy Correction = 0.307739

Atomic No	x-coord	y-coord	z-coord
7	-0.578647	-1.619942	1.094536
6	-1.881064	-1.768826	1.443661
6	-2.874362	-0.987889	0.920667
1	-2.120498	-2.553548	2.169297
1	-3.907045	-1.120178	1.231275
6	0.382403	-2.504397	1.463444

6	1.650796	-2.462847	0.954129
1	0.104171	-3.273600	2.191744
1	2.403784	-3.176202	1.277359
15	-2.391391	0.182582	-0.356428
15	1.967625	-1.239492	-0.325957
8	0.952544	2.450362	0.925483
6	-3.152070	1.811500	0.097456
1	-2.950705	2.547111	-0.688586
1	-4.237228	1.717058	0.221903
1	-2.718747	2.172413	1.034299
6	-3.341961	-0.227996	-1.886550
1	-4.422330	-0.203875	-1.701918
1	-3.093633	0.490294	-2.675039
1	-3.046763	-1.225040	-2.220001
6	3.533217	-0.371896	0.158943
1	4.343077	-1.090550	0.330633
1	3.840475	0.318755	-0.634049
1	3.366267	0.198623	1.076592
6	2.526213	-2.143428	-1.837382
1	2.762999	-1.424864	-2.629097
1	3.410915	-2.756517	-1.629167
1	1.708811	-2.781003	-2.180687
77	-0.076991	-0.102695	-0.388105
6	0.383758	1.261532	1.028653
6	0.127149	1.021656	2.499523
1	-0.434143	-1.213450	-1.586708
1	0.240296	0.908203	-1.602496
1	-0.927808	0.767743	2.651572
1	0.695704	0.137766	2.811885
1	0.403528	1.880866	3.120308
6	1.343853	3.000101	-0.358733
6	2.015217	4.334111	-0.086488
1	0.447249	3.099106	-0.974460
1	2.007852	2.286857	-0.850903
1	2.323928	4.789893	-1.033742
1	1.331825	5.023783	0.419776
1	2.904105	4.208494	0.540550

Structure 8-13TS - DEE

B3LYP/GBS(1) = -1390.293636 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.590126 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.379763 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.666496 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.719593 a.u.
Enthalpy Correction = 0.379918
Gibbs Free Energy Correction = 0.302951
Imaginary Freq = -852.3i

Atomic No	x-coord	y-coord	z-coord
7	-1.118228	-1.931664	0.312277
6	-2.474237	-1.974041	0.369764
6	-3.255839	-0.877439	0.160670
1	-2.928715	-2.944739	0.591129
1	-4.338690	-0.941119	0.217084
6	-0.370854	-3.051282	0.479391

6	0.986600	-3.040555	0.368151
1	-0.905317	-3.978535	0.708108
1	1.576643	-3.939546	0.519088
15	-2.402966	0.657751	-0.200319
15	1.737205	-1.454406	0.005677
8	1.826320	2.057743	0.697680
6	-3.205405	1.929070	0.892735
1	-2.775171	2.920688	0.719450
1	-4.279526	1.969277	0.676995
1	-3.071597	1.662725	1.943563
6	-3.019173	1.252947	-1.845441
1	-4.113002	1.323616	-1.853220
1	-2.597050	2.238919	-2.069657
1	-2.698625	0.550502	-2.618413
6	2.978833	-1.204503	1.361082
1	3.659869	-2.062050	1.412622
1	3.566809	-0.294136	1.214849
1	2.439035	-1.121526	2.307639
6	2.835356	-1.732446	-1.462731
1	3.426067	-0.837842	-1.684716
1	3.518015	-2.571009	-1.282815
1	2.207945	-1.962767	-2.327812
77	-0.135071	-0.032314	-0.181237
6	0.624142	1.446324	0.840754
6	-0.027786	2.195000	1.990148
1	-0.406808	-0.521557	-1.913290
1	0.120934	0.364437	-1.811485
1	-0.913232	1.684130	2.359659
1	0.694898	2.286930	2.811259
1	-0.289970	3.219439	1.686202
6	2.622461	1.929836	-0.487223
6	3.298192	3.269782	-0.739000
1	1.973193	1.626799	-1.314514
1	3.372712	1.146855	-0.332417
1	3.946955	3.200566	-1.619822
1	2.553652	4.052051	-0.919203
1	3.911173	3.569433	0.117438

Structure 9 -DEE

B3LYP/GBS(1) = -1390.347129 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.645129 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.449052 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.72223757 a.u.
Enthalpy Correction = 0.384391
Gibbs Free Energy Correction = 0.309852

Atomic No	x-coord	y-coord	z-coord
7	-1.103554	-1.697003	-0.833294
6	-2.404404	-1.612424	-1.219811
6	-3.184402	-0.524891	-0.964125
1	-2.808081	-2.475349	-1.755269
1	-4.220156	-0.487048	-1.286774
6	-0.364699	-2.817941	-1.063974
6	0.928621	-2.945130	-0.660463
1	-0.868057	-3.628584	-1.596579
1	1.493900	-3.849367	-0.864097

15	-2.390399	0.796069	-0.053024
15	1.621247	-1.527311	0.191518
8	2.128644	1.973333	0.267740
6	-3.421494	1.130174	1.447204
1	-3.014535	1.979871	2.007183
1	-4.458904	1.355355	1.174420
1	-3.396637	0.245094	2.087416
6	-2.634982	2.356384	-1.019397
1	-3.698094	2.541023	-1.212005
1	-2.226742	3.213653	-0.471502
1	-2.105386	2.262873	-1.970659
6	2.294602	-2.125696	1.807226
1	3.010381	-2.942256	1.658317
1	2.802242	-1.306700	2.328574
1	1.464482	-2.475656	2.425224
6	3.177813	-1.081906	-0.699194
1	3.658994	-0.241669	-0.190873
1	3.869248	-1.931940	-0.731239
1	2.927320	-0.782567	-1.720044
77	-0.235776	-0.092210	0.210499
6	0.802527	1.854523	0.610690
6	0.456145	1.217573	1.819187
1	0.163689	0.475495	-1.322089
1	0.175432	2.651200	0.212579
6	2.364207	2.458385	-1.053355
6	3.835749	2.814923	-1.183305
1	1.738344	3.346662	-1.232309
1	2.060848	1.691415	-1.778840
1	4.039890	3.202798	-2.187548
1	4.116590	3.580057	-0.452083
1	4.469917	1.937236	-1.021309
1	-0.767288	-0.910166	1.572150
1	-0.385045	1.591826	2.392764
1	1.247295	0.774044	2.415778

Structure 10 - DEE

B3LYP/GBS(1) = -1390.351287 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.647107 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.447875 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.721789 a.u.
Enthalpy Correction = 0.385187
Gibbs Free Energy Correction = 0.308802

Atomic No	x-coord	y-coord	z-coord
7	0.002611	0.419765	1.586216
6	-1.033366	1.048192	2.199970
6	-2.278250	1.138994	1.640776
1	-0.837488	1.486504	3.184339
1	-3.079233	1.662183	2.155915
6	1.179809	0.152390	2.215344
6	2.147822	-0.637631	1.664737
1	1.326934	0.599898	3.204053
1	3.081351	-0.816138	2.191514
15	-2.527244	0.272413	0.083190
15	1.763997	-1.406249	0.079570
8	1.689469	1.883032	-0.970575

6	-3.350430	1.468360	-1.073413
1	-3.616033	0.959942	-2.006877
1	-4.262991	1.877082	-0.624674
1	-2.677966	2.298618	-1.307661
6	-3.899204	-0.939756	0.343039
1	-4.805194	-0.445613	0.712741
1	-4.125129	-1.446792	-0.601107
1	-3.570541	-1.687499	1.068697
6	3.191593	-1.072825	-1.050115
1	4.136150	-1.376358	-0.583866
1	3.063884	-1.634754	-1.982009
1	3.220931	-0.005340	-1.276863
6	1.921119	-3.232626	0.322216
1	1.738481	-3.744699	-0.628503
1	2.918120	-3.501872	0.689796
1	1.166952	-3.558135	1.042555
77	-0.379798	-0.565880	-0.309768
6	0.391311	1.554519	-1.242875
1	-0.346652	2.259687	-0.868240
6	1.870075	2.903609	0.020303
6	3.358742	3.057217	0.274388
1	1.341180	2.620001	0.935153
1	1.437559	3.844455	-0.353301
1	3.535248	3.863681	0.994854
1	3.771775	2.129685	0.682604
1	3.888525	3.300043	-0.652771
6	0.081032	0.633925	-2.225806
1	0.880512	0.161570	-2.785886
1	-0.879488	0.691772	-2.721467
1	-0.768077	-1.584836	-1.507608
1	-0.861186	-1.821619	0.579031

Structure 10b - DEE

B3LYP/GBS(1) = -1390.354866 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.651896 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.452730 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.727083 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.775025 a.u.
Enthalpy Correction = 0.385197
Gibbs Free Energy Correction = 0.30944

Atomic No	x-coord	y-coord	z-coord
7	1.239961	1.616520	-0.766176
6	0.572336	2.774348	-1.010695
6	-0.725486	2.968480	-0.633643
1	1.124144	3.566003	-1.527412
1	-1.232789	3.903618	-0.853875
6	2.561838	1.458107	-1.025388
6	3.257181	0.337911	-0.661863
1	3.068486	2.278503	-1.543752
1	4.314109	0.241147	-0.893512
15	-1.513636	1.627160	0.270746
15	2.342922	-0.911515	0.248711
8	-2.200389	-1.763813	-0.876388
6	-3.161603	1.353509	-0.529103
1	-3.741913	0.632761	0.054503

1	-3.715432	2.297851	-0.585328
1	-3.033789	0.952199	-1.536257
6	-2.037947	2.305883	1.909608
1	-2.695233	3.175003	1.790214
1	-2.565697	1.531683	2.476880
1	-1.145846	2.598036	2.468600
6	2.682215	-2.532134	-0.590785
1	3.761228	-2.700987	-0.683802
1	2.249031	-3.354598	-0.010705
1	2.243146	-2.538529	-1.592700
6	3.206679	-1.174354	1.861654
1	2.708573	-1.972469	2.422272
1	4.258814	-1.442064	1.710826
1	3.146326	-0.251503	2.443542
77	0.202933	0.032510	0.276311
6	-0.849257	-1.653020	-1.021811
1	-0.288191	-2.550208	-0.767088
6	-2.637834	-2.599924	0.196413
6	-4.136668	-2.806580	0.059494
1	-2.377214	-2.122397	1.149703
1	-2.107168	-3.563448	0.148208
1	-4.503078	-3.445236	0.870733
1	-4.667708	-1.850226	0.108738
1	-4.379428	-3.283815	-0.895581
6	-0.309615	-0.680308	-1.850790
1	-0.966904	0.027170	-2.344701
1	0.646395	-0.853627	-2.330560
1	-0.450806	-0.979153	1.364407
1	0.678210	0.749707	1.644631

Structure 10b-16TS - DEE

B3LYP/GBS(1) = -1390.31731 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.612780 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.411437 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.688837 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.736836 a.u.
Enthalpy Correction = 0.381488
Gibbs Free Energy Correction = 0.306724
Imaginary Freq = -132.9i

Atomic No	x-coord	y-coord	z-coord
7	-0.430245	-1.077865	1.578223
6	-1.602425	-0.935728	2.251068
6	-2.689805	-0.313721	1.706912
1	-1.647938	-1.346863	3.264219
1	-3.616830	-0.213536	2.263631
6	0.642843	-1.700395	2.139190
6	1.828667	-1.857140	1.482908
1	0.517646	-2.081120	3.157483
1	2.664847	-2.364587	1.955309
15	-2.482279	0.309642	0.038085
15	1.903573	-1.206481	-0.190375
8	1.586265	2.203469	-0.373772
6	-3.077288	2.066048	0.049433
1	-3.030861	2.494286	-0.957927

1	-4.113050	2.114568	0.403864
1	-2.450917	2.664778	0.716133
6	-3.794678	-0.478046	-1.009543
1	-4.792822	-0.304667	-0.591128
1	-3.758713	-0.068615	-2.025033
1	-3.614104	-1.555145	-1.060140
6	3.497578	-0.280632	-0.332459
1	4.340915	-0.952264	-0.134111
1	3.600397	0.139508	-1.337164
1	3.510613	0.540623	0.383751
6	2.270742	-2.648432	-1.302831
1	2.396139	-2.302798	-2.334868
1	3.185887	-3.162644	-0.987686
1	1.437785	-3.355486	-1.268977
77	-0.248803	-0.260420	-0.412035
6	0.329717	1.749324	-0.756220
1	-0.449768	2.451416	-0.448370
6	1.645065	2.653729	0.975256
6	2.941334	3.422270	1.181185
1	1.574408	1.792322	1.656030
1	0.781776	3.306219	1.185367
1	3.007821	3.781975	2.214261
1	3.813038	2.789600	0.982901
1	2.989517	4.284872	0.508345
6	0.187532	1.070798	-2.023764
1	1.099660	0.874630	-2.585336
1	-0.648752	1.357444	-2.660465
1	-0.785279	-1.728988	-1.560036
1	-0.927095	-2.221763	-0.953170

Structure 11 - DEE

B3LYP/GBS(1) = -1390.306107 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.605587 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.399835 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.679601 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.729941 a.u.
Enthalpy Correction = 0.383467
Gibbs Free Energy Correction = 0.306236

Atomic No	x-coord	y-coord	z-coord
7	-1.883332	0.472319	-1.189881
6	-2.060971	1.770572	-1.566024
6	-1.342918	2.796476	-1.033014
1	-2.826502	1.959985	-2.323556
1	-1.500236	3.819459	-1.361933
6	-2.724266	-0.515165	-1.609074
6	-2.676233	-1.785530	-1.119529
1	-3.461459	-0.239129	-2.368185
1	-3.351672	-2.552565	-1.486337
15	-0.143722	2.359136	0.232793
15	-1.460000	-2.087951	0.166102
8	3.668823	-0.934393	-0.228164
6	-0.573351	3.304352	1.762650
1	0.175025	3.110773	2.538626
1	-0.615600	4.381731	1.565324
1	-1.544211	2.957520	2.122652

6	1.416555	3.225459	-0.273016
1	1.222278	4.295833	-0.408378
1	2.191905	3.105485	0.490901
1	1.780321	2.812882	-1.217355
6	-2.347761	-2.715131	1.658488
1	-2.940694	-3.606317	1.423165
1	-1.622169	-2.962152	2.440615
1	-3.003727	-1.924609	2.029477
6	-0.505034	-3.588906	-0.347037
1	0.223133	-3.862048	0.424020
1	-1.184310	-4.433991	-0.505007
1	0.027367	-3.386698	-1.280042
77	-0.445254	0.018500	0.314113
6	2.626966	0.017886	-0.378899
6	1.284195	-0.634393	-0.296827
1	2.703632	0.502873	-1.374129
1	2.727750	0.821184	0.367038
1	1.451072	-1.712636	-0.423096
6	4.962585	-0.373501	-0.354655
6	5.989845	-1.481394	-0.183492
1	5.113968	0.413912	0.404597
1	5.073538	0.107846	-1.342821
1	7.005499	-1.080799	-0.276114
1	5.888323	-1.948844	0.801340
1	5.849944	-2.254905	-0.945729
1	0.211838	-0.163590	1.784416
1	-1.719531	0.391070	1.347434

Structure 11-15TS - DEE

B3LYP/GBS(1) = -1390.279236 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.581414 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.373263 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.654552 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.707792 a.u.
Enthalpy Correction = 0.380079
Gibbs Free Energy Correction = 0.302696
Imaginary Freq = -783.8i

Atomic No	x-coord	y-coord	z-coord
7	-2.164239	0.577762	-0.885556
6	-2.331414	1.881703	-1.224619
6	-1.465838	2.857700	-0.829334
1	-3.203252	2.126271	-1.838981
1	-1.622293	3.893339	-1.117356
6	-3.020277	-0.395869	-1.288570
6	-2.860534	-1.708089	-0.948911
1	-3.864220	-0.083836	-1.911364
1	-3.564142	-2.462614	-1.288075
15	-0.044992	2.342914	0.142325
15	-1.440279	-2.103029	0.072232
8	3.671078	-0.945948	-0.193090
6	-0.086854	3.316185	1.718823
1	0.807844	3.106851	2.315058
1	-0.136205	4.392030	1.515539
1	-0.968054	3.020540	2.294005

6	1.403507	3.134283	-0.703016
1	1.205510	4.202109	-0.852183
1	2.314851	3.026310	-0.107153
1	1.557695	2.665638	-1.678287
6	-2.069313	-2.938892	1.599187
1	-2.690748	-3.805717	1.347088
1	-1.228048	-3.270377	2.217064
1	-2.667258	-2.225684	2.172706
6	-0.545306	-3.492385	-0.758960
1	0.289307	-3.838254	-0.140075
1	-1.225837	-4.333272	-0.933120
1	-0.151932	-3.146449	-1.718249
77	-0.438187	0.010594	0.312541
6	2.629701	0.014674	-0.308349
6	1.295595	-0.656638	-0.123473
1	2.670588	0.486168	-1.309840
1	2.782093	0.820541	0.427966
1	1.459051	-1.729601	-0.281018
6	4.961148	-0.394847	-0.369809
6	5.988518	-1.506102	-0.219302
1	5.143353	0.400858	0.374549
1	5.042801	0.074854	-1.366638
1	7.002796	-1.112586	-0.350488
1	5.917126	-1.960988	0.774094
1	5.819336	-2.288357	-0.966593
1	-0.678496	0.101961	1.975196
1	-1.604970	0.379131	1.643784

Structure 12 - DEE

B3LYP/GBS(1) = -1390.316020 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.615243 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1389.409525 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1390.687837 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1390.73829 a.u.
Enthalpy Correction = 0.382717
Gibbs Free Energy Correction = 0.304546

Atomic No	x-coord	y-coord	z-coord
7	2.447245	0.701742	-0.272822
6	2.656609	2.035502	-0.406108
6	1.679193	2.958187	-0.174983
1	3.657754	2.354403	-0.711528
1	1.873256	4.020454	-0.290498
6	3.420592	-0.215759	-0.498517
6	3.216327	-1.558100	-0.355979
1	4.399572	0.164147	-0.806047
1	4.014603	-2.269582	-0.543943
15	0.069957	2.332697	0.313428
15	1.576796	-2.064761	0.158357
8	-3.520742	-0.915220	1.397569
6	-1.148804	3.054442	-0.879642
1	-2.173239	2.796382	-0.589783
1	-1.059561	4.146469	-0.915992

1	-0.951272	2.642644	-1.872279
6	-0.386408	3.209908	1.878750
1	-0.326423	4.297074	1.751803
1	-1.406278	2.947742	2.181135
1	0.303612	2.898942	2.666906
6	0.948966	-3.295512	-1.070205
1	1.626175	-4.153097	-1.156069
1	-0.040254	-3.656312	-0.767315
1	0.858103	-2.804416	-2.041966
6	1.753923	-3.107482	1.674891
1	0.770361	-3.461831	2.002587
1	2.397701	-3.975047	1.489351
1	2.186801	-2.496024	2.470201
77	0.483270	0.004320	0.340785
6	-2.476679	0.018421	1.191287
6	-1.194702	-0.691297	0.866589
1	-2.324754	0.633503	2.098343
1	-2.736795	0.716048	0.376361
1	-1.354442	-1.772226	0.988097
6	-4.762194	-0.308543	1.708777
6	-5.798324	-1.403107	1.908265
1	-5.068487	0.370402	0.893616
1	-4.666744	0.305963	2.621376
1	-6.774097	-0.967458	2.149965
1	-5.900728	-2.003647	0.998606
1	-5.501344	-2.067409	2.726296
1	1.165150	0.201647	1.855755
1	0.237445	0.005460	-1.314467

Structure 13 - DEE

B3LYP/GBS(1) = -1389.155554 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.440371 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.228140 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.510424 a.u.
Enthalpy Correction = 0.36697
Gibbs Free Energy Correction = 0.287908

Atomic No	x-coord	y-coord	z-coord
7	0.310343	-2.145946	-0.532020
6	-0.773905	-2.942970	-0.732502
6	-2.049934	-2.506027	-0.525566
1	-0.584366	-3.965299	-1.073988
1	-2.906049	-3.152240	-0.693363
6	1.567041	-2.619848	-0.749476
6	2.679387	-1.853974	-0.555306
1	1.656919	-3.656000	-1.090013
1	3.676593	-2.244800	-0.732965
15	-2.190500	-0.812336	0.034994
15	2.363706	-0.182061	0.000039
8	-0.229024	2.842425	0.238157
6	-3.175484	-0.833040	1.605977
1	-3.336364	0.191080	1.960034
1	-4.148874	-1.314755	1.456227

1	-2.617562	-1.383131	2.368215
6	-3.380138	0.035172	-1.108761
1	-4.326270	-0.515556	-1.169374
1	-3.586713	1.051928	-0.756806
1	-2.936048	0.091293	-2.106091
6	3.358463	0.076892	1.543838
1	4.417413	-0.151376	1.374560
1	3.270123	1.116049	1.879655
1	2.972289	-0.578183	2.329104
6	3.254185	0.945625	-1.174505
1	3.174496	1.985061	-0.837888
1	4.315232	0.678021	-1.242934
1	2.801141	0.859452	-2.165608
77	0.033557	-0.110912	0.145436
6	-0.207970	1.654615	0.858688
6	-0.399964	1.937144	2.338228
1	-0.437570	1.007627	2.907228
1	0.428949	2.554581	2.710224
1	-1.321588	2.511576	2.503771
6	-0.084982	2.902095	-1.199754
6	-1.189438	3.778447	-1.766393
1	-0.114039	1.876870	-1.584873
1	0.902353	3.334497	-1.398898
1	-1.057907	3.889801	-2.848844
1	-2.172644	3.331154	-1.585203
1	-1.175276	4.775947	-1.314166

Structure 14 - DEE

B3LYP/GBS(1) = -232.4257127 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -232.509465 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -232.344179 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -232.539701 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -232.498677 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -232.3314557 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -231.852384 a.u.
Enthalpy Correction = 0.120823
Gibbs Free Energy Correction = 0.082331

Atomic No	x-coord	y-coord	z-coord
6	2.299807	-0.350987	-0.022457
6	1.070145	0.535930	0.064814
1	3.209488	0.254981	0.050045
1	2.303616	-1.083352	0.791007
1	2.316325	-0.893035	-0.973334
1	1.053619	1.086981	1.016840
1	1.063441	1.274684	-0.750870
6	-1.282612	0.348020	-0.045140
6	-2.448934	-0.294864	0.026878
8	-0.084692	-0.298692	-0.030814
1	-3.377684	0.261766	-0.014137
1	-2.495988	-1.375080	0.118111
1	-1.225712	1.433996	-0.135721

Structure 15 - DEE
B3LYP/GBS(1) = -1389.123657 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.411151 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.207180 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.478906 a.u.
Enthalpy Correction = 0.366356
Gibbs Free Energy Correction = 0.287456

Atomic No	x-coord	y-coord	z-coord
7	2.394877	0.713532	-0.039700
6	2.626193	2.067513	-0.048142
6	1.617482	2.977956	-0.031078
1	3.670727	2.391907	-0.069397
1	1.821298	4.044566	-0.038904
6	3.438268	-0.179755	-0.057915
6	3.248749	-1.526676	-0.045288
1	4.448172	0.239980	-0.083157
1	4.089221	-2.213766	-0.059590
15	-0.051520	2.293459	-0.002189
15	1.528781	-2.057953	0.000934
8	-3.724143	-0.994128	-0.024322
6	-0.925716	3.072435	-1.439684
1	-1.982323	2.783119	-1.444257
1	-0.857162	4.165623	-1.397872
1	-0.465546	2.719118	-2.366335
6	-0.898168	3.103967	1.433976
1	-0.827719	4.195936	1.369694
1	-1.954884	2.817562	1.459333
1	-0.424887	2.767642	2.360346
6	1.279993	-3.216603	-1.421525
1	1.971520	-4.065314	-1.370117
1	0.252167	-3.594660	-1.416023
1	1.444721	-2.672944	-2.355469
6	1.355358	-3.198121	1.449585
1	0.331346	-3.583309	1.498675
1	2.049497	-4.043183	1.376815
1	1.561088	-2.640353	2.366955
77	0.413416	-0.010739	0.011819
6	-2.665530	-0.061361	0.117577
6	-1.329638	-0.744295	0.054897
1	-2.752114	0.466031	1.088812
1	-2.736653	0.716079	-0.665203
1	-1.514626	-1.830094	0.055179
6	-5.006862	-0.401502	0.039117
6	-6.053774	-1.491604	-0.129231
1	-5.114514	0.362123	-0.751867
1	-5.140636	0.117043	1.005442
1	-7.062453	-1.065733	-0.086383
1	-5.929292	-1.996047	-1.092997
1	-5.958033	-2.240441	0.663834

Structure 16 - DEE
B3LYP/GBS(1) = -1389.156221 a.u.

B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.443597 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.24492 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.515051 a.u.
Enthalpy Correction = 0.367059
Gibbs Free Energy Correction = 0.291183

Atomic No	x-coord	y-coord	z-coord
7	0.921806	-1.686947	-0.923621
6	2.230825	-1.695352	-1.331983
6	3.102822	-0.695771	-1.029286
1	2.552398	-2.557537	-1.922517
1	4.133783	-0.723402	-1.368067
6	0.099387	-2.748432	-1.211971
6	-1.188307	-2.816812	-0.783365
1	0.535513	-3.554423	-1.808309
1	-1.819054	-3.666187	-1.027209
15	2.409614	0.625273	-0.028932
15	-1.734503	-1.410092	0.197276
8	-1.900633	2.114223	0.260974
6	2.781196	2.210760	-0.917949
1	2.447067	3.068070	-0.322487
1	3.855410	2.315127	-1.108713
1	2.247082	2.218821	-1.871974
6	3.491186	0.789437	1.467556
1	4.537912	0.954919	1.188041
1	3.153614	1.630655	2.083157
1	3.417572	-0.126291	2.060163
6	-3.306435	-0.814015	-0.574432
1	-4.068678	-1.601737	-0.579985
1	-3.673441	0.051256	-0.015806
1	-3.105416	-0.505875	-1.603905
6	-2.357000	-2.093812	1.803502
1	-2.796473	-1.292096	2.406639
1	-3.116462	-2.866192	1.637643
1	-1.517619	-2.525643	2.354958
77	0.209247	-0.110281	0.235241
6	-0.608515	1.841888	0.684702
1	0.099427	2.617737	0.381355
6	-1.981484	2.602535	-1.076514
6	-3.401617	3.078801	-1.335523
1	-1.689644	1.810325	-1.779792
1	-1.271115	3.435586	-1.205320
1	-3.485928	3.481500	-2.351260
1	-4.116555	2.255992	-1.233132
1	-3.680489	3.864808	-0.625916
6	-0.407830	1.126593	1.887781
1	-1.280833	0.765053	2.426899
1	0.430274	1.393395	2.529238

1.7. Coordinates of DEE structures at the Full-opt level of Theory

Full Structure 1
B3LYP/GBS(1) = -1858.308996 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1858.721264 a.u.

M06/GBS(2)//B3LYP/GBS(1) = -1857.737816 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -1854.284379 a.u.
Enthalpy Correction = 0.660821
Gibbs Free Energy Correction = 0.555111

Atomic No	x-coord	y-coord	z-coord
1	-5.190014	4.358114	-1.326943
1	-5.939098	3.013545	-0.452540
6	-5.103116	3.721466	-0.438165
1	-5.243039	4.371834	0.436410
1	-2.612669	4.674928	-1.108283
6	-2.579615	3.649657	-0.743590
6	-3.773995	3.005168	-0.395505
1	-3.102969	-0.165254	-2.619928
1	-3.401024	-1.809830	-3.210497
1	-5.201607	-0.518741	-1.097938
1	-0.458602	3.562530	-0.950340
6	-1.343525	3.020588	-0.641025
6	-3.671911	1.661426	-0.024576
1	-4.583668	1.115181	0.203344
6	-2.877680	-1.223078	-2.445084
1	-5.349300	-2.190730	-1.639545
1	2.885383	-0.703361	-4.005625
6	-4.861972	-1.540577	-0.901783
1	-1.800805	-1.369318	-2.572972
1	2.378664	0.588181	-2.899789
1	1.339568	-0.826494	-3.140096
6	2.380032	-0.495306	-3.054047
6	-2.444576	0.991064	0.047772
6	-1.222288	1.691081	-0.173364
1	-5.224459	-1.839523	0.087246
6	-3.336687	-1.662300	-1.044857
1	0.458579	3.562536	0.950303
1	5.243037	4.371824	-0.436426
1	-3.060066	-2.717552	-0.916990
1	2.612640	4.674941	1.108256
6	1.343505	3.020595	0.640996
7	-0.000005	1.014477	-0.000014
6	2.579592	3.649668	0.743567
15	-2.282713	-0.821697	0.271314
6	1.222275	1.691085	0.173340
1	3.587468	-2.964033	-3.123535
6	3.093991	-1.232348	-1.910167
1	-4.127609	-0.864611	1.851522
1	4.127676	-0.864632	-1.851444
6	3.773977	3.005180	0.395497
6	5.103096	3.721482	0.438164
1	2.098234	-3.153814	-2.178337
6	2.444566	0.991071	-0.047783
1	5.189973	4.358155	1.326926
6	3.116194	-2.749710	-2.156223
6	3.671899	1.661436	0.024574
6	-3.093922	-1.232328	1.910209
1	5.939080	3.013563	0.452577
1	4.583661	1.115189	-0.203329
1	-2.378560	0.588222	2.899768
15	2.282714	-0.821691	-0.271312
1	-3.677855	-3.292345	1.388363
1	3.677908	-3.292353	-1.388256

6	-2.379913	-0.495263	3.054043
6	-3.116114	-2.749685	2.156297
1	-2.885218	-0.703306	4.005648
1	-3.587352	-2.963988	3.123631
1	-1.339443	-0.826443	3.140046
1	-2.098153	-3.153788	2.178384
1	5.224443	-1.839560	-0.087136
1	5.201568	-0.518714	1.097977
6	3.336645	-1.662267	1.044911
6	4.861933	-1.540559	0.901869
1	3.060019	-2.717521	0.917070
1	3.102908	-0.165168	2.619927
1	1.800729	-1.369215	2.572978
6	2.877609	-1.222994	2.445112
1	5.349239	-2.190675	1.639677
1	3.400926	-1.809728	3.210557
77	-0.000002	-1.067653	-0.000021
1	-0.069641	-2.413312	-0.856331
1	0.069640	-2.413321	0.856276

Full Structure 2

B3LYP/GBS(1) = -1857.063574 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1857.464228 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1856.490182 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -1853.022693 a.u.
Enthalpy Correction = 0.64345
Gibbs Free Energy Correction = 0.538759

Atomic No	x-coord	y-coord	z-coord
1	-5.127007	4.197765	-1.677187
1	-5.886318	3.008416	-0.609072
6	-5.036654	3.692784	-0.707099
1	-5.148589	4.465429	0.065960
1	-2.510639	4.590242	-1.308015
6	-2.503961	3.577999	-0.907195
6	-3.722347	2.959454	-0.580312
1	-3.261974	-0.418834	-2.551981
1	-3.522383	-2.115870	-2.996529
1	-5.267122	-0.675427	-0.881813
1	-0.377256	3.451739	-1.040523
6	-1.284111	2.936711	-0.747563
6	-3.655575	1.632791	-0.153373
1	-4.582675	1.111902	0.071680
6	-2.993552	-1.451117	-2.301656
1	-5.412838	-2.377318	-1.320792
1	2.742713	-0.424130	-4.079050
6	-4.901009	-1.679496	-0.645585
1	-1.915596	-1.565657	-2.456771
1	2.372256	0.807905	-2.857391
1	1.239407	-0.524215	-3.133558
6	2.301677	-0.259708	-3.087535
6	-2.440746	0.946554	-0.012448
6	-1.205546	1.618352	-0.232819
1	-5.211155	-1.925918	0.375101
6	-3.381886	-1.786981	-0.852360
1	0.377246	3.451851	1.040134

1	5.148674	4.465322	-0.066339
1	-3.087967	-2.829509	-0.661231
1	2.510629	4.590363	1.307586
6	1.284105	2.936786	0.747253
7	0.000002	0.951221	-0.000073
6	2.503957	3.578081	0.906863
15	-2.274600	-0.831438	0.343292
6	1.205547	1.618380	0.232642
1	3.418453	-2.757154	-3.410581
6	3.030179	-1.114409	-2.039254
1	-4.077740	-0.786837	1.988905
1	4.077596	-0.786991	-1.988973
6	3.722347	2.959493	0.580086
6	5.036659	3.692818	0.706849
1	1.953320	-2.967798	-2.436525
6	2.440748	0.946553	0.012362
1	5.126943	4.197971	1.676854
6	2.987981	-2.604760	-2.412908
6	3.655578	1.632788	0.153269
77	0.000005	-1.057268	0.000116
6	-3.030331	-1.114264	2.039281
1	5.886317	3.008414	0.609014
1	4.582683	1.111868	-0.071693
1	-2.372422	0.808087	2.857344
15	2.274597	-0.831473	-0.343216
1	-3.551223	-3.230677	1.711876
1	3.551063	-3.230810	-1.711757
6	-2.301899	-0.259513	3.087571
6	-2.988178	-2.604595	2.413027
1	-2.743034	-0.423850	4.079055
1	-3.418718	-2.756922	3.410681
1	-1.239642	-0.524051	3.133714
1	-1.953524	-2.967646	2.436737
1	5.211134	-1.926009	-0.375256
1	5.267278	-0.675387	0.881520
6	3.382009	-1.786903	0.852398
6	4.901110	-1.679472	0.645439
1	3.088046	-2.829444	0.661410
1	3.262329	-0.418578	2.551895
1	1.915903	-1.565367	2.456948
6	2.993846	-1.450878	2.301704
1	5.412998	-2.377236	1.320662
1	3.522728	-2.115579	2.996587

Full Structure 3 - DEE

B3LYP/GBS(1) = -2090.734578 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2091.215651 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2090.083375 a.u.
Enthalpy Correction = 0.789804
Gibbs Free Energy Correction = 0.666642

Atomic No	x-coord	y-coord	z-coord
8	-1.630241	-3.852406	-0.268204

77	-0.044612	-0.557144	0.137413
6	-0.529926	-3.413906	0.472093
6	-0.539301	-4.074080	1.842814
1	-0.619250	-2.289247	0.687394
1	0.409836	-3.607119	-0.054496
1	0.276376	-3.682437	2.458580
1	-1.487037	-3.882108	2.354424
1	-0.417938	-5.157133	1.735737
6	-1.493096	-3.670953	-1.677038
6	-2.762648	-4.160463	-2.352028
1	-0.621732	-4.244219	-2.033517
1	-1.300925	-2.608376	-1.888364
1	-2.674936	-4.058667	-3.439254
1	-2.944339	-5.214204	-2.115594
1	-3.629484	-3.579925	-2.020535
15	-2.178402	0.227089	0.566416
6	-2.010286	1.942895	-0.020993
6	-3.582398	-0.583027	-0.406748
6	-2.804700	0.344489	2.334979
6	-3.068719	2.844209	-0.202208
6	-0.684312	2.304189	-0.382246
6	-3.366179	-0.340107	-1.910463
6	-5.022519	-0.236773	0.003929
1	-3.420792	-1.651695	-0.207990
1	-3.779271	0.849826	2.295501
6	-1.847970	1.196390	3.182900
6	-2.989311	-1.052049	2.949164
6	-2.895021	4.091240	-0.803925
1	-4.065416	2.561034	0.127086
6	-0.528677	3.538102	-1.063129
7	0.367496	1.422859	-0.119060
1	-3.576893	0.701883	-2.173186
1	-4.037035	-0.979491	-2.498236
1	-2.332955	-0.553491	-2.203853
1	-5.261191	0.813522	-0.192559
1	-5.725223	-0.841942	-0.583690
1	-5.222329	-0.440013	1.060535
1	-1.759903	2.214121	2.790793
1	-2.215654	1.259041	4.215256
1	-0.845352	0.754832	3.199268
1	-3.678694	-1.680302	2.373733
1	-3.388482	-0.968782	3.967971
1	-2.026742	-1.572523	3.007880
6	-4.040598	5.059659	-0.981031
6	-1.601235	4.396096	-1.259414
1	0.442698	3.811646	-1.457544
6	1.683702	1.862810	0.018874
1	-4.119677	5.410011	-2.018228
1	-4.997440	4.598169	-0.713687
1	-3.920834	5.952197	-0.351814
1	-1.430277	5.329754	-1.792902
6	2.045630	3.192177	0.358195
6	2.753196	0.935225	-0.122972
1	1.272544	3.913796	0.592565
6	3.373628	3.588258	0.418734
6	4.085144	1.373573	-0.093735
15	2.228289	-0.802882	-0.251960
1	3.596884	4.619902	0.686177
6	4.431655	2.701727	0.155873
1	4.880678	0.652818	-0.264822
6	2.928905	-1.405742	-1.892996

6	3.156394	-1.794794	1.062393
6	5.869313	3.164842	0.168026
6	2.309281	-0.600664	-3.045664
1	4.008588	-1.203900	-1.870458
6	2.711820	-2.912354	-2.094681
6	4.673987	-1.962059	0.886055
1	2.697006	-2.790911	0.977635
6	2.821452	-1.241895	2.457700
1	6.094318	3.820966	-0.684075
1	6.105359	3.732630	1.077251
1	6.561662	2.317315	0.117991
1	2.732302	-0.927069	-4.004553
1	2.501219	0.471012	-2.935943
1	1.223460	-0.743692	-3.078930
1	3.131233	-3.229460	-3.057855
1	1.642311	-3.150854	-2.106710
1	3.187237	-3.516965	-1.314358
1	4.949789	-2.348995	-0.100412
1	5.199970	-1.014987	1.041175
1	5.054543	-2.669907	1.633861
1	3.252452	-0.244022	2.596404
1	1.738448	-1.159077	2.598561
1	3.233899	-1.898820	3.234487

Full Structure 3-5TS - DEE

B3LYP/GBS(1) = -2090.723015 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2091.208696 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2090.077813 a.u.
Enthalpy Correction = 0.785878
Gibbs Free Energy Correction = 0.664872
Imaginary Freq = -725.6i

Atomic No	x-coord	y-coord	z-coord
8	-1.322655	-3.376403	-0.684673
77	-0.006670	-0.671021	0.139827
6	-0.218756	-3.050613	0.121355
6	-0.273417	-4.005419	1.323661
1	-0.166529	-1.971950	1.092342
1	0.713280	-3.227961	-0.417946
1	0.573247	-3.835006	1.998153
1	-1.198555	-3.864917	1.892807
1	-0.244706	-5.042532	0.969891
6	-1.137110	-3.153058	-2.080012
6	-2.288992	-3.802546	-2.829492
1	-0.182149	-3.603456	-2.396721
1	-1.072350	-2.074182	-2.273317
1	-2.168792	-3.653496	-3.908587
1	-2.321580	-4.878819	-2.629153
1	-3.247558	-3.369317	-2.528844
15	-2.174749	-0.018680	0.664207
6	-2.190660	1.676572	-0.019484
6	-3.664531	-0.924539	-0.076303
6	-2.569472	0.157988	2.495853
6	-3.334752	2.472675	-0.164315
6	-0.937484	2.119213	-0.517035

6	-3.782405	-0.624077	-1.580702
6	-5.021812	-0.724808	0.619492
1	-3.373583	-1.976644	0.029878
1	-3.586784	0.566875	2.557375
6	-1.609142	1.151837	3.166680
6	-2.534487	-1.203662	3.207907
6	-3.319704	3.684721	-0.857891
1	-4.274472	2.131746	0.263194
6	-0.946208	3.305735	-1.289425
7	0.208898	1.345473	-0.284491
1	-4.136829	0.395894	-1.758446
1	-4.499870	-1.314369	-2.041778
1	-2.824033	-0.734886	-2.096233
1	-5.372140	0.310969	0.554872
1	-5.776079	-1.350731	0.125046
1	-5.004724	-1.010806	1.675040
1	-1.675096	2.145648	2.713579
1	-1.854943	1.246085	4.232338
1	-0.572058	0.810780	3.081166
1	-3.204468	-1.939892	2.749697
1	-2.835836	-1.088470	4.256832
1	-1.520228	-1.617176	3.192675
6	-4.555924	4.542799	-0.990153
6	-2.101967	4.059318	-1.447402
1	-0.036040	3.625713	-1.783392
6	1.466552	1.938058	-0.154112
1	-4.728851	4.847102	-2.030147
1	-5.449769	4.010473	-0.647211
1	-4.476969	5.464362	-0.397295
1	-2.058333	4.962338	-2.054045
6	1.686968	3.323433	0.061841
6	2.629628	1.117782	-0.168424
1	0.841787	3.985667	0.201173
6	2.966466	3.857501	0.121782
6	3.909792	1.690126	-0.147264
15	2.309984	-0.676139	-0.129424
1	3.075048	4.927868	0.289962
6	4.115780	3.064564	-0.023131
1	4.779893	1.042466	-0.220029
6	3.226733	-1.328150	-1.644460
6	3.241520	-1.402192	1.346355
6	5.499938	3.669176	-0.024110
6	2.605054	-0.743734	-2.922616
1	4.253378	-0.947334	-1.557180
6	3.284571	-2.861877	-1.712990
6	4.777313	-1.400047	1.283959
1	2.903371	-2.448596	1.351243
6	2.750547	-0.743414	2.646269
1	5.631938	4.382032	0.799671
1	6.271939	2.898462	0.077953
1	5.706685	4.215967	-0.954591
1	3.166760	-1.080866	-3.803286
1	2.614620	0.350310	-2.912144
1	1.564800	-1.069130	-3.036152
1	3.900404	-3.173790	-2.566045
1	2.287224	-3.290512	-1.860774
1	3.716231	-3.313453	-0.813362
1	5.172078	-1.855674	0.370219
1	5.176269	-0.384234	1.360900
1	5.176949	-1.969750	2.132803
1	3.055378	0.308184	2.689846

1	1.659335	-0.780352	2.718622
1	3.182531	-1.256972	3.514788

Full Structure 4 - DEE

B3LYP/GBS(1) = -2090.735204 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2091.217122 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2090.082130 a.u.
Enthalpy Correction = 0.790495
Gibbs Free Energy Correction = 0.668385

Atomic No	x-coord	y-coord	z-coord
8	3.686898	-2.784937	0.036362
77	0.067769	-0.536055	0.064980
6	2.539958	-3.605071	-0.076888
6	1.300482	-2.867111	0.423025
1	2.674534	-4.515152	0.533112
1	2.404527	-3.933049	-1.121456
1	0.478976	-3.578566	0.521530
1	1.492212	-2.400647	1.390532
1	1.015518	-2.124357	-0.403645
6	4.878407	-3.457044	-0.347777
6	6.069008	-2.546517	-0.095494
1	4.823623	-3.741009	-1.412091
1	4.981237	-4.389757	0.232304
1	6.998716	-3.055190	-0.373392
1	5.991162	-1.627572	-0.685300
1	6.126885	-2.272827	0.963013
15	1.881238	0.848755	-0.329952
6	1.122862	2.463896	0.047669
6	3.367428	0.609366	0.805412
6	2.583833	1.021757	-2.065351
6	1.819581	3.669746	0.205626
6	-0.283094	2.411925	0.247058
6	2.929855	0.794861	2.268417
6	4.635483	1.421278	0.497724
1	3.600947	-0.451894	0.656407
1	3.347020	1.810693	-2.020572
6	1.481654	1.464638	-3.039921
6	3.239033	-0.284123	-2.540544
6	1.195867	4.844310	0.630480
1	2.886546	3.694565	-0.000681
6	-0.896694	3.587819	0.746493
7	-0.966844	1.216191	0.011400
1	2.707196	1.845162	2.486488
1	3.731163	0.470744	2.944910
1	2.029662	0.210614	2.488615
1	4.491108	2.491681	0.676998
1	5.448154	1.091563	1.158360
1	4.981451	1.291959	-0.533089
1	1.058997	2.433825	-2.758910
1	1.890631	1.551538	-4.054901
1	0.665400	0.733821	-3.057403
1	4.002121	-0.653121	-1.848356
1	3.711280	-0.133889	-3.519937
1	2.484056	-1.071339	-2.649363
6	1.955788	6.140789	0.784174

6	-0.174317	4.758984	0.926918
1	-1.946599	3.570991	1.014049
6	-2.329783	1.190737	-0.282704
1	1.759159	6.613373	1.754956
1	3.036774	5.980864	0.706547
1	1.677714	6.871576	0.012132
1	-0.690017	5.633712	1.320047
6	-3.042821	2.284620	-0.836768
6	-3.067181	-0.009309	-0.083400
1	-2.509319	3.187595	-1.108244
6	-4.409913	2.217473	-1.062425
6	-4.454472	-0.034869	-0.285554
15	-2.044425	-1.444968	0.373210
1	-4.909061	3.083270	-1.494815
6	-5.162373	1.069820	-0.760670
1	-5.002564	-0.948863	-0.072084
6	-2.666297	-1.977178	2.068622
6	-2.482261	-2.876404	-0.780287
6	-6.658689	1.033092	-0.963876
6	-2.485433	-0.827452	3.072014
1	-3.740774	-2.183324	1.966439
6	-1.960255	-3.249557	2.561386
6	-3.858659	-3.536794	-0.604496
1	-1.718322	-3.625920	-0.526940
6	-2.254279	-2.451397	-2.240566
1	-7.183105	1.693131	-0.259323
1	-6.940159	1.358730	-1.973712
1	-7.055520	0.022117	-0.820171
1	-2.857998	-1.127722	4.059907
1	-3.030773	0.068632	2.760559
1	-1.427318	-0.559405	3.167984
1	-2.351383	-3.542076	3.544000
1	-0.883915	-3.075672	2.672603
1	-2.100439	-4.100862	1.885485
1	-4.054111	-3.845365	0.427422
1	-4.666897	-2.870340	-0.921043
1	-3.917705	-4.435330	-1.232533
1	-2.997002	-1.708320	-2.551011
1	-1.261987	-2.007073	-2.372230
1	-2.345778	-3.319610	-2.905992

Full Structure 4-6TS - DEE

B3LYP/GBS(1) = -2090.730605 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2091.217533 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2090.081353 a.u.
Enthalpy Correction = 0.785919
Gibbs Free Energy Correction = 0.663419
Imaginary Freq = -692.9i

Atomic No	x-coord	y-coord	z-coord
8	-1.913183	-3.898885	-0.400745
77	-0.113416	-0.473210	0.295639
6	-2.035499	-3.312798	0.883879
6	-0.791793	-2.481163	1.181402
1	-2.140245	-4.104086	1.647744

1	-2.944328	-2.691170	0.932586
1	-0.915018	-2.013725	2.162576
1	0.071575	-3.147483	1.212746
1	-0.749574	-1.933531	-0.118386
6	-3.006557	-4.729331	-0.751314
6	-2.774773	-5.273557	-2.151747
1	-3.947859	-4.154525	-0.710403
1	-3.100830	-5.555395	-0.025310
1	-3.602486	-5.926571	-2.450069
1	-2.699456	-4.454520	-2.874303
1	-1.845410	-5.851183	-2.189878
15	2.064185	-1.134299	-0.133127
6	2.906968	0.480321	-0.180231
6	2.898973	-2.161178	1.215094
6	2.458908	-2.019329	-1.740727
6	4.296299	0.654478	-0.256879
6	2.044670	1.599309	-0.011807
6	2.834602	-1.409305	2.555113
6	4.322959	-2.668587	0.936312
1	2.243339	-3.039789	1.291576
1	3.553601	-2.080936	-1.812475
6	1.937213	-1.201067	-2.931630
6	1.875503	-3.442124	-1.745282
6	4.905251	1.898486	-0.085857
1	4.926416	-0.209964	-0.449520
6	2.676759	2.839701	0.257084
7	0.657794	1.415395	-0.046123
1	3.472452	-0.518903	2.535707
1	3.183984	-2.057958	3.368466
1	1.814101	-1.084794	2.782869
1	5.047016	-1.848118	0.926246
1	4.627461	-3.358369	1.734166
1	4.404194	-3.209997	-0.011784
1	2.376398	-0.198747	-2.956313
1	2.188746	-1.707014	-3.872566
1	0.848925	-1.091018	-2.877549
1	2.294569	-4.069043	-0.950176
1	2.097451	-3.933655	-2.700995
1	0.787024	-3.423071	-1.622166
6	6.400996	2.077564	-0.196446
6	4.057438	2.976348	0.216738
1	2.072555	3.700378	0.517871
6	-0.208305	2.453209	-0.400343
1	6.802061	2.662258	0.641003
1	6.919103	1.112306	-0.205357
1	6.681640	2.606475	-1.117771
1	4.491276	3.951532	0.432050
6	0.180639	3.619287	-1.108948
6	-1.596740	2.334423	-0.110334
1	1.196859	3.711588	-1.471195
6	-0.716698	4.644283	-1.374033
6	-2.471001	3.404255	-0.350384
15	-2.120303	0.690480	0.482659
1	-0.362778	5.516029	-1.922235
6	-2.057843	4.588076	-0.963153
1	-3.513833	3.309440	-0.058789
6	-2.944098	1.026608	2.142656
6	-3.512510	0.091098	-0.645882
6	-3.005568	5.740671	-1.196940
6	-1.916403	1.611662	3.124342
1	-3.712495	1.788421	1.953768

6	-3.624378	-0.217769	2.732900
6	-4.845173	0.855052	-0.592299
1	-3.693485	-0.929479	-0.281591
6	-2.997179	-0.015079	-2.090804
1	-4.043474	5.449641	-1.001111
1	-2.778186	6.595425	-0.545030
1	-2.952837	6.106128	-2.230436
1	-2.400681	1.849694	4.080107
1	-1.464038	2.528599	2.734551
1	-1.108921	0.896402	3.317438
1	-4.123555	0.040510	3.675382
1	-2.892025	-1.002176	2.956596
1	-4.382150	-0.642328	2.065419
1	-5.235970	0.967364	0.424547
1	-4.752695	1.851071	-1.035836
1	-5.600022	0.311045	-1.174726
1	-2.772479	0.976092	-2.500267
1	-2.085213	-0.617573	-2.140124
1	-3.760992	-0.478740	-2.728250

Full Structure 5 - DEE

B3LYP/GBS(1) = -2090.750284 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2091.23433648 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2090.100336 a.u.
MP2/GBS(2)//B3LYP/GBS(1)
Enthalpy Correction = 0.78735
Gibbs Free Energy Correction = 0.66691

Atomic No	x-coord	y-coord	z-coord
8	1.602217	-3.262641	-0.619108
77	0.048618	-0.665686	-0.072564
6	0.346865	-2.618853	-0.880754
6	0.224167	-2.567144	-2.403838
1	0.387193	-1.645918	1.107210
1	-0.438562	-3.291209	-0.498605
1	-0.740245	-2.153622	-2.708399
1	1.011047	-1.953225	-2.850530
1	0.312207	-3.578277	-2.827663
6	1.685303	-3.951563	0.606094
6	3.008087	-4.703754	0.661894
1	0.842176	-4.658104	0.702845
1	1.606636	-3.245394	1.451800
1	3.097101	-5.253240	1.606117
1	3.080501	-5.418029	-0.164996
1	3.853818	-4.011422	0.585654
15	-2.222207	-0.846569	0.396860
6	-2.789953	0.861363	0.068216
6	-3.281897	-1.975450	-0.693810
6	-2.703763	-1.254036	2.164451
6	-4.137191	1.244829	0.033743
6	-1.766916	1.776730	-0.303298
6	-3.421594	-1.379931	-2.106796
6	-4.660059	-2.387805	-0.149823
1	-2.666033	-2.881969	-0.768847
1	-3.799518	-1.191182	2.206662
6	-2.121458	-0.217832	3.138011

6	-2.269116	-2.677936	2.548696
6	-4.548468	2.494085	-0.436713
1	-4.895432	0.540904	0.368677
6	-2.198311	3.001807	-0.866662
7	-0.422009	1.397624	-0.168345
1	-4.130436	-0.546322	-2.113341
1	-3.791105	-2.146671	-2.798778
1	-2.470267	-1.003935	-2.494215
1	-5.336187	-1.531214	-0.058244
1	-5.127540	-3.093333	-0.848725
1	-4.604357	-2.882795	0.823829
1	-2.470335	0.793819	2.909526
1	-2.426108	-0.459820	4.164161
1	-1.027175	-0.214801	3.097408
1	-2.674634	-3.441822	1.876287
1	-2.613624	-2.912801	3.563492
1	-1.177774	-2.765135	2.533028
6	-6.002219	2.904335	-0.442530
6	-3.543956	3.343364	-0.924857
1	-1.464829	3.684954	-1.278548
6	0.587864	2.340978	0.067249
1	-6.285370	3.375914	-1.391523
1	-6.661530	2.042900	-0.289465
1	-6.223380	3.629087	0.353076
1	-3.821807	4.298267	-1.367793
6	0.361051	3.678900	0.476376
6	1.950996	1.937307	-0.018032
1	-0.647758	4.014093	0.680855
6	1.405292	4.578840	0.648928
6	2.980927	2.878340	0.118413
15	2.257033	0.140056	-0.208500
1	1.169858	5.594513	0.962868
6	2.742185	4.218369	0.431290
1	4.010357	2.555451	-0.013131
6	3.383584	0.053363	-1.717603
6	3.341902	-0.394071	1.241868
6	3.863378	5.224072	0.545319
6	2.658919	0.596184	-2.960131
1	4.206956	0.744827	-1.490944
6	3.979964	-1.342228	-1.960162
6	4.790973	0.120586	1.259687
1	3.363588	-1.484908	1.121885
6	2.651252	-0.068773	2.576888
1	3.911972	5.882155	-0.333405
1	3.737625	5.871513	1.421865
1	4.837006	4.729651	0.634231
1	3.349378	0.615217	-3.812693
1	2.291573	1.614557	-2.799183
1	1.804704	-0.029890	-3.235520
1	4.588488	-1.326090	-2.873482
1	3.207704	-2.106651	-2.067587
1	4.630853	-1.657511	-1.137557
1	5.329187	-0.064666	0.325302
1	4.830042	1.193379	1.472141
1	5.343327	-0.387066	2.060826
1	2.584392	1.014260	2.728993
1	1.638848	-0.479340	2.617054
1	3.230962	-0.490319	3.407974

Full Structure 5-9TS - DEE

B3LYP/GBS(1) = -2090.719771 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2091.21125 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2090.075340 a.u.
Enthalpy Correction = 0.782277
Gibbs Free Energy Correction = 0.664218
Imaginary Freq = -762.4i

Atomic No	x-coord	y-coord	z-coord
8	-1.753500	-3.355090	-0.781486
77	-0.001964	-0.697666	0.362309
6	-0.537043	-2.900833	-0.338288
6	-0.364591	-2.683219	1.081566
1	-0.458846	-1.513509	-1.135695
1	0.301923	-3.331636	-0.881518
6	-1.830169	-3.587010	-2.190244
6	-3.126115	-4.319129	-2.491162
1	-0.964344	-4.189149	-2.505165
1	-1.776937	-2.624424	-2.718607
1	-3.206428	-4.511602	-3.566558
1	-3.159695	-5.277423	-1.962979
1	-3.990883	-3.724295	-2.182317
1	0.439674	-0.025013	1.771711
1	0.503245	-3.163632	1.531191
1	-1.265434	-2.810207	1.679442
15	-2.118733	0.181485	0.824320
6	-2.066615	1.738125	-0.125877
6	-3.639002	-0.784769	0.240480
6	-2.503372	0.660398	2.602856
6	-3.190877	2.546429	-0.354713
6	-0.804756	2.077476	-0.688316
6	-3.778945	-0.682254	-1.286959
6	-4.977507	-0.468110	0.928417
1	-3.371208	-1.821571	0.474065
1	-3.529121	1.051754	2.592222
6	-1.576181	1.775607	3.106416
6	-2.445036	-0.565903	3.528025
6	-3.153104	3.665246	-1.186232
1	-4.133520	2.287768	0.121998
6	-0.795355	3.174057	-1.591331
7	0.309255	1.305370	-0.396150
1	-4.145102	0.303763	-1.587974
1	-4.494430	-1.432960	-1.644822
1	-2.823300	-0.847212	-1.791612
1	-5.303357	0.561753	0.746127
1	-5.755252	-1.128228	0.523072
1	-4.948105	-0.627248	2.010196
1	-1.643755	2.671112	2.481606
1	-1.856868	2.051558	4.130968
1	-0.532360	1.446231	3.115535
1	-3.119427	-1.368839	3.208598
1	-2.729621	-0.281427	4.548869
1	-1.429246	-0.972959	3.558462
6	-4.368080	4.533857	-1.412239
6	-1.930149	3.935334	-1.824946
1	0.115974	3.405663	-2.130589
6	1.585881	1.824794	-0.336989

1	-4.566405	4.684648	-2.481197
1	-5.265065	4.087695	-0.969000
1	-4.245137	5.530957	-0.967667
1	-1.869897	4.760310	-2.533093
6	1.896267	3.214543	-0.303785
6	2.701547	0.939701	-0.234560
1	1.091781	3.937732	-0.255566
6	3.202908	3.672874	-0.302206
6	4.014694	1.436597	-0.277734
15	2.316236	-0.828827	-0.035704
1	3.376818	4.747602	-0.272826
6	4.303743	2.798471	-0.329083
1	4.843758	0.734716	-0.262735
6	3.056674	-1.601416	-1.595697
6	3.359184	-1.563615	1.362763
6	5.721800	3.315263	-0.384115
6	2.339684	-1.067453	-2.844799
1	4.090131	-1.229476	-1.620471
6	3.106225	-3.137992	-1.596835
6	4.879650	-1.654645	1.135487
1	2.967976	-2.590079	1.425137
6	3.070091	-0.870465	2.703357
1	5.940705	3.810523	-1.340165
1	5.918095	4.051233	0.406626
1	6.446420	2.502186	-0.264836
1	2.815073	-1.466384	-3.750115
1	2.379117	0.024668	-2.892064
1	1.284518	-1.360846	-2.852244
1	3.669632	-3.488789	-2.470862
1	2.104718	-3.575079	-1.668149
1	3.589522	-3.553203	-0.706841
1	5.152605	-2.097267	0.173086
1	5.351645	-0.669949	1.204421
1	5.324203	-2.279465	1.920529
1	3.362943	0.184965	2.668915
1	2.010040	-0.917099	2.960072
1	3.646453	-1.356096	3.501173

Full Structure 6 - DEE

B3LYP/GBS(1) = -2090.747203 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2091.23123 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2090.096400 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -2086.1658739 a.u.
Enthalpy Correction = 0.788289
Gibbs Free Energy Correction = 0.669903

Atomic No	x-coord	y-coord	z-coord
8	0.665279	-2.142352	1.740202
77	-0.010211	-0.880686	-0.282900
6	0.404126	-3.385677	1.029508
6	0.124946	-2.994933	-0.424655
1	-0.456811	-3.873547	1.507662
1	1.277022	-4.042113	1.171145

1	0.937355	-3.331153	-1.080260
1	-0.788690	-3.484476	-0.782770
1	-0.347655	-0.587938	-1.772498
6	0.663965	-2.243819	3.160263
6	1.043988	-0.901347	3.763395
1	1.381639	-3.022869	3.462905
1	-0.331911	-2.564263	3.506126
1	0.990252	-0.952156	4.856844
1	2.061325	-0.616784	3.479270
1	0.366970	-0.114501	3.416746
15	2.179715	-0.334657	-0.895637
6	2.392679	1.236721	0.019201
6	3.621731	-1.503460	-0.527393
6	2.415661	0.103500	-2.712302
6	3.631138	1.828053	0.303388
6	1.178108	1.846630	0.462652
6	3.865263	-1.628397	0.985190
6	4.943192	-1.257982	-1.277660
1	3.219115	-2.465817	-0.874679
1	3.465429	0.411272	-2.804714
6	1.543521	1.295116	-3.133993
6	2.169365	-1.115111	-3.616777
6	3.751809	2.990257	1.067866
1	4.537983	1.363367	-0.074145
6	1.318131	2.997293	1.282278
7	-0.032856	1.249992	0.143967
1	4.280110	-0.704256	1.401039
1	4.582608	-2.436272	1.178997
1	2.935682	-1.853545	1.510850
1	5.404849	-0.303593	-1.003992
1	5.657069	-2.048881	-1.013471
1	4.826417	-1.276475	-2.364892
1	1.752979	2.181899	-2.528764
1	1.745612	1.543589	-4.183766
1	0.477610	1.067213	-3.037414
1	2.819546	-1.962249	-3.371243
1	2.355403	-0.848772	-4.664940
1	1.132126	-1.456699	-3.532883
6	5.095152	3.616737	1.359795
6	2.561698	3.542175	1.569129
1	0.433716	3.444209	1.721601
6	-1.230395	1.930833	0.047366
1	5.242917	3.780522	2.435181
1	5.915621	2.982367	1.006933
1	5.204723	4.594669	0.871372
1	2.611275	4.419201	2.212861
6	-1.348852	3.341650	-0.100006
6	-2.456378	1.195774	0.013009
1	-0.451511	3.942457	-0.186266
6	-2.581801	3.969790	-0.171498
6	-3.688900	1.867163	-0.028022
15	-2.326636	-0.627910	0.000024
1	-2.608957	5.052069	-0.290348
6	-3.790851	3.255408	-0.105901
1	-4.606102	1.283095	-0.006999
6	-3.335921	-1.167135	1.502463
6	-3.336284	-1.285547	-1.469997
6	-5.126482	3.960054	-0.139853
6	-2.835255	-0.491667	2.786672
1	-4.356200	-0.807496	1.315593
6	-3.373031	-2.694884	1.656418

6	-4.863773	-1.352055	-1.291379
1	-2.958204	-2.311978	-1.575143
6	-3.005600	-0.527435	-2.766683
1	-5.290410	4.570244	0.758999
1	-5.209055	4.635714	-1.001305
1	-5.953059	3.243684	-0.202546
1	-3.465683	-0.788849	3.634687
1	-2.865369	0.598707	2.706902
1	-1.806886	-0.785238	3.015997
1	-4.023469	-2.974774	2.494823
1	-2.373396	-3.087802	1.864892
1	-3.748289	-3.203672	0.762276
1	-5.174008	-1.932710	-0.418589
1	-5.305935	-0.353302	-1.212378
1	-5.307605	-1.830357	-2.173803
1	-3.318973	0.520024	-2.702088
1	-1.937119	-0.548117	-2.992915
1	-3.537947	-0.989699	-3.607571

Full Structure 7 - DEE

B3LYP/GBS(1) = -2090.741847 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2091.230243 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2090.088626 a.u.
Enthalpy Correction = 0.784167
Gibbs Free Energy Correction = 0.66597

Atomic No	x-coord	y-coord	z-coord
8	-0.473382	-3.666790	-0.192575
77	-0.010462	-0.721416	0.182975
6	-0.038172	-2.639616	0.534905
6	0.458466	-3.270138	1.826792
1	-0.327198	-0.866615	-1.462803
1	0.312982	-0.470783	1.812450
1	1.039311	-2.565819	2.417129
1	-0.416904	-3.568706	2.419296
1	1.030581	-4.184106	1.623972
6	-1.001246	-3.575838	-1.536053
6	-0.579070	-4.831031	-2.280800
1	-0.638585	-2.653866	-1.992513
1	-2.090418	-3.518231	-1.452751
1	-1.009385	-4.820604	-3.288559
1	0.510511	-4.886158	-2.374300
1	-0.926933	-5.733686	-1.767519
15	-2.264832	-0.171314	0.545345
6	-2.344364	1.515934	-0.131949
6	-3.570324	-1.222407	-0.337622
6	-2.880647	-0.037941	2.318463
6	-3.546973	2.196159	-0.375901
6	-1.091084	2.115598	-0.441300
6	-3.531820	-0.978111	-1.855497
6	-5.014058	-1.134103	0.188509
1	-3.214900	-2.243029	-0.145856
1	-3.934196	0.262856	2.243389

6	-2.123570	1.053679	3.088434
6	-2.793125	-1.386327	3.048751
6	-3.587495	3.446528	-0.991448
1	-4.486188	1.731962	-0.086140
6	-1.149716	3.355134	-1.136025
7	0.074116	1.448788	-0.117651
1	-3.966672	-0.005164	-2.104720
1	-4.115684	-1.751080	-2.371749
1	-2.509016	-0.992927	-2.241246
1	-5.446264	-0.138760	0.044705
1	-5.642289	-1.840103	-0.369678
1	-5.098135	-1.390946	1.248315
1	-2.250819	2.035901	2.623903
1	-2.503745	1.110191	4.116533
1	-1.052745	0.830030	3.126213
1	-3.319320	-2.191676	2.522736
1	-3.234511	-1.302322	4.049757
1	-1.746325	-1.682928	3.167136
6	-4.887640	4.175812	-1.234847
6	-2.354588	3.989117	-1.394462
1	-0.232388	3.804336	-1.497468
6	1.288684	2.088291	0.026532
1	-4.986215	4.493484	-2.280945
1	-5.749994	3.542353	-0.999294
1	-4.969867	5.081530	-0.618343
1	-2.341046	4.933430	-1.936679
6	1.445179	3.469244	0.331419
6	2.492177	1.332122	-0.063878
1	0.566059	4.072014	0.525533
6	2.695431	4.059569	0.418975
6	3.744189	1.963783	-0.004947
15	2.291694	-0.470179	-0.214206
1	2.755447	5.119644	0.661080
6	3.882363	3.332916	0.217336
1	4.644266	1.367059	-0.127860
6	2.993321	-0.917207	-1.900757
6	3.457776	-1.304032	1.024955
6	5.234806	4.003788	0.262188
6	2.322516	-0.096548	-3.011676
1	4.054717	-0.637959	-1.862678
6	2.886304	-2.423578	-2.184076
6	4.935391	-1.431954	0.612315
1	3.045875	-2.319547	1.094537
6	3.347067	-0.652367	2.413403
1	5.385076	4.678501	-0.591897
1	5.359265	4.608103	1.170081
1	6.045806	3.267453	0.241977
1	2.752353	-0.369114	-3.984143
1	2.471450	0.976843	-2.862222
1	1.244927	-0.287487	-3.040033
1	3.362160	-2.660225	-3.144011
1	1.836971	-2.728341	-2.248091
1	3.369675	-3.037551	-1.415733
1	5.073410	-1.951141	-0.340183
1	5.427546	-0.456703	0.543531
1	5.471071	-2.007228	1.378151
1	3.806768	0.341344	2.416554
1	2.305235	-0.538258	2.724216
1	3.870481	-1.270576	3.153758

Full Structure 8-13TS - DEE

B3LYP/GBS(1) = -2090.673643 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2091.163976 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2090.030130 a.u.
Enthalpy Correction = 0.779441
Gibbs Free Energy Correction = 0.660983
Imaginary Freq = -922.3i

Atomic No	x-coord	y-coord	z-coord
7	0.060928	1.378039	-0.232865
6	1.257214	2.062782	-0.164355
6	2.480223	1.329510	-0.160337
6	-1.144903	2.007123	-0.481584
6	-2.362363	1.407691	-0.051683
15	2.342341	-0.474707	0.018388
15	-2.272165	-0.299404	0.574177
8	-0.590684	-3.392682	-0.974274
6	3.517312	-1.009043	1.414822
1	3.178965	-2.030464	1.633805
6	3.143522	-1.169545	-1.538692
1	4.170048	-0.779318	-1.530218
6	-2.993818	-0.257549	2.322290
1	-4.064749	-0.060445	2.190997
6	-3.594575	-1.281027	-0.401361
1	-3.178146	-2.295330	-0.411719
77	0.038634	-0.759333	0.421796
6	0.027960	-2.690592	-0.013252
6	0.635732	-3.745746	0.898927
1	1.416708	-3.324985	1.532825
1	-0.157994	-4.114162	1.564354
1	1.017910	-4.606691	0.337097
6	-1.065010	-2.792765	-2.194637
6	-0.455741	-3.540260	-3.371393
1	-0.798250	-1.731323	-2.168766
1	-2.151567	-2.892218	-2.202466
1	-0.866156	-3.145789	-4.308168
1	0.631698	-3.421059	-3.397985
1	-0.686020	-4.609643	-3.319547
1	0.236973	-1.132284	2.046477
1	0.199979	-0.052448	2.045731
6	-3.586016	2.081587	-0.204433
6	-1.282848	3.207703	-1.235115
6	-2.508625	3.829797	-1.405956
1	-2.552287	4.745006	-1.994423
6	-3.692818	3.309635	-0.853331
1	-4.491913	1.620461	0.183922
1	-0.409568	3.635387	-1.712407
6	1.390282	3.473054	-0.010448
6	3.717370	1.992975	-0.214535
6	2.626465	4.097724	-0.021699
1	2.664015	5.179348	0.099617
6	3.826871	3.381158	-0.173966
1	0.505879	4.077436	0.145488
1	4.630009	1.406162	-0.278013
6	-2.422703	0.879110	3.182014
1	-1.346200	0.762519	3.340981
1	-2.591190	1.857354	2.722217

1	-2.912279	0.874567	4.164571
6	-2.827143	-1.617953	3.019851
1	-1.769149	-1.826295	3.210380
1	-3.350554	-1.615744	3.984291
1	-3.226530	-2.448818	2.426864
6	-3.697354	-0.773804	-1.852496
1	-4.194727	-1.526581	-2.477752
1	-4.289213	0.144398	-1.901432
1	-2.722847	-0.549076	-2.292728
6	-5.006139	-1.377207	0.205413
1	-5.485605	-0.396155	0.294077
1	-5.638395	-1.983876	-0.456118
1	-5.017926	-1.852327	1.189994
6	3.304113	-0.161172	2.679351
1	3.642270	0.868527	2.522976
1	2.254207	-0.127228	2.978934
1	3.882986	-0.586296	3.508943
6	5.019200	-1.082512	1.083083
1	5.448371	-0.088825	0.923194
1	5.550516	-1.526160	1.934759
1	5.241504	-1.696859	0.206481
6	3.200254	-2.703405	-1.547131
1	2.193649	-3.131332	-1.546493
1	3.711105	-3.054391	-2.452707
1	3.737619	-3.114405	-0.685788
6	2.441756	-0.626580	-2.791458
1	2.920890	-1.029324	-3.693106
1	1.384883	-0.910858	-2.802777
1	2.491666	0.465118	-2.835955
6	-5.010844	4.034899	-0.986236
1	-5.049217	4.932696	-0.353771
1	-5.189594	4.365317	-2.017479
1	-5.850412	3.394836	-0.693054
6	5.161556	4.082859	-0.257579
1	5.288134	4.610203	-1.213386
1	5.276591	4.832433	0.535952
1	5.991825	3.373758	-0.165619

Full Structure 13 - DEE

B3LYP/GBS(1) = -2089.55426 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2090.032172 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2088.906413 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -2084.995625 a.u.
Enthalpy Correction = 0.766774
Gibbs Free Energy Correction = 0.647942

Atomic No	x-coord	y-coord	z-coord
8	-0.349286	-3.648054	-0.342240
77	-0.004660	-0.738568	0.146886
6	-0.008798	-2.629878	0.469517
6	0.404630	-3.285946	1.778348
1	0.678662	-2.541309	2.525440
1	-0.417311	-3.902895	2.164207
1	1.252154	-3.964623	1.610460
6	-0.711739	-3.398870	-1.716374
6	-0.278866	-4.597063	-2.545190

1	-0.239192	-2.462640	-2.029491
1	-1.797398	-3.269973	-1.760424
1	-0.584990	-4.456100	-3.588014
1	0.808383	-4.724479	-2.521080
1	-0.739793	-5.518545	-2.173735
15	-2.262845	-0.252552	0.485584
6	-2.387175	1.479618	-0.061323
6	-3.524197	-1.241761	-0.523746
6	-2.922670	-0.277396	2.246065
6	-3.602448	2.161077	-0.224274
6	-1.152471	2.095653	-0.411027
6	-3.373700	-0.914920	-2.019793
6	-5.000561	-1.152923	-0.099208
1	-3.196482	-2.277237	-0.361937
1	-3.952756	0.101086	2.193103
6	-2.101709	0.674014	3.130110
6	-2.942090	-1.695198	2.837542
6	-3.679785	3.424361	-0.810488
1	-4.522475	1.688320	0.109634
6	-1.253891	3.339161	-1.092664
7	0.034923	1.431808	-0.135671
1	-3.757843	0.086183	-2.239221
1	-3.943519	-1.634975	-2.621296
1	-2.328292	-0.944945	-2.341287
1	-5.415637	-0.155164	-0.270842
1	-5.591562	-1.854613	-0.702156
1	-5.159089	-1.412660	0.951455
1	-2.132620	1.701099	2.754415
1	-2.498442	0.671235	4.153511
1	-1.052312	0.361341	3.164850
1	-3.511132	-2.404748	2.226386
1	-3.397571	-1.679515	3.835807
1	-1.923570	-2.082352	2.941889
6	-4.991395	4.158658	-0.958199
6	-2.473337	3.972632	-1.278467
1	-0.360323	3.796875	-1.499421
6	1.240831	2.108030	-0.036660
1	-5.130470	4.540178	-1.977862
1	-5.841745	3.506424	-0.730002
1	-5.054526	5.023932	-0.283746
1	-2.491558	4.922772	-1.810336
6	1.379874	3.497361	0.237933
6	2.459492	1.377432	-0.143870
1	0.499061	4.086380	0.462655
6	2.618517	4.119513	0.250186
6	3.696873	2.039729	-0.169126
15	2.291781	-0.431993	-0.120451
1	2.663200	5.186074	0.465970
6	3.811516	3.418927	0.000172
1	4.603749	1.458843	-0.317897
6	3.217959	-1.050973	-1.634035
6	3.299187	-1.049880	1.355336
6	5.145415	4.125072	-0.055379
6	2.559283	-0.511769	-2.913107
1	4.231708	-0.633106	-1.568223
6	3.319066	-2.583463	-1.656560
6	4.829691	-0.954331	1.248092
1	3.028428	-2.112469	1.410301
6	2.804377	-0.364492	2.640108
1	5.243078	4.745398	-0.957167
1	5.288670	4.791242	0.805141

1	5.975455	3.409893	-0.061666
1	3.120327	-0.846377	-3.795107
1	2.533095	0.582083	-2.920420
1	1.527741	-0.869802	-3.006195
1	3.850645	-2.913459	-2.558022
1	2.324684	-3.041842	-1.668051
1	3.859792	-2.981390	-0.791104
1	5.227769	-1.439967	0.351345
1	5.167583	0.086580	1.253576
1	5.285726	-1.447228	2.116471
1	3.079979	0.695533	2.646753
1	1.715095	-0.424689	2.728973
1	3.258988	-0.838907	3.519220

Full Structure 16 - DEE

B3LYP/GBS(1) = -2089.555248 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2090.035959 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2088.914471 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -2085.004453 a.u.
Enthalpy Correction = 0.767169
Gibbs Free Energy Correction = 0.650064

Atomic No	x-coord	y-coord	z-coord
8	0.665606	-3.470450	-0.919675
77	-0.008521	-0.718227	0.295881
6	-0.171975	-2.846400	-0.003825
1	-1.216544	-3.111182	-0.175903
6	0.125699	-3.555109	-2.236988
6	1.017869	-4.452707	-3.078885
1	0.047276	-2.549808	-2.673979
1	-0.892491	-3.973227	-2.186747
1	0.599968	-4.558852	-4.086400
1	2.025675	-4.035525	-3.168313
1	1.096834	-5.447923	-2.629033
6	0.273521	-2.604479	1.318491
1	1.305655	-2.844263	1.561131
1	-0.418991	-2.763789	2.141939
15	-2.287005	-0.377729	0.673826
6	-2.553890	1.181338	-0.239315
6	-3.529840	-1.643730	0.019357
6	-2.845157	-0.018224	2.434852
6	-3.805596	1.716061	-0.570893
6	-1.358943	1.807487	-0.683526
6	-3.456559	-1.703549	-1.516285
6	-4.988275	-1.537941	0.496088
1	-3.133157	-2.590412	0.412980
1	-3.907127	0.254451	2.366060
6	-2.077453	1.181605	3.011073
6	-2.703256	-1.247257	3.346064
6	-3.947016	2.826211	-1.406628
1	-4.703620	1.248887	-0.176185
6	-1.512147	2.882950	-1.592060
7	-0.123165	1.291795	-0.271859
1	-3.890923	-0.804306	-1.964621
1	-4.016538	-2.571823	-1.885817
1	-2.424002	-1.782371	-1.869711

1	-5.482329	-0.639688	0.113514
1	-5.553904	-2.400080	0.119538
1	-5.080737	-1.539552	1.586122
1	-2.224553	2.083301	2.409115
1	-2.426105	1.391550	4.030313
1	-1.002852	0.974873	3.052033
1	-3.229638	-2.127621	2.960054
1	-3.114044	-1.027004	4.339384
1	-1.648632	-1.512346	3.473408
6	-5.301807	3.404257	-1.741680
6	-2.766604	3.369670	-1.936231
1	-0.633982	3.325833	-2.046733
6	1.016808	2.098567	-0.217231
1	-5.412986	3.577525	-2.819413
1	-6.110311	2.734845	-1.428144
1	-5.467145	4.370180	-1.244829
1	-2.829818	4.195002	-2.643512
6	0.990826	3.515460	-0.147567
6	2.300443	1.491635	-0.147532
1	0.040378	4.029960	-0.076149
6	2.157616	4.266831	-0.149781
6	3.462162	2.276728	-0.193563
15	2.306653	-0.317556	0.101501
1	2.078434	5.351496	-0.095793
6	3.427046	3.671548	-0.216482
1	4.431694	1.785711	-0.202015
6	3.476499	-0.957625	-1.226948
6	3.226759	-0.634122	1.723209
6	4.687296	4.501506	-0.284575
6	2.875916	-0.718035	-2.620396
1	4.382846	-0.342838	-1.140457
6	3.858604	-2.430888	-1.014920
6	4.711190	-0.238204	1.770971
1	3.165707	-1.725392	1.832056
6	2.460470	0.001451	2.894358
1	4.795818	5.000253	-1.257523
1	4.696024	5.289178	0.479544
1	5.579706	3.884176	-0.134005
1	3.585253	-1.039114	-3.393966
1	2.650828	0.340301	-2.786422
1	1.948492	-1.283296	-2.751877
1	4.501903	-2.768486	-1.838071
1	2.968905	-3.065616	-0.990674
1	4.415366	-2.585110	-0.084199
1	5.293828	-0.651659	0.941656
1	4.832026	0.849122	1.768151
1	5.156123	-0.612451	2.702001
1	2.457536	1.094473	2.812150
1	1.421426	-0.340447	2.916655
1	2.940233	-0.263319	3.845426

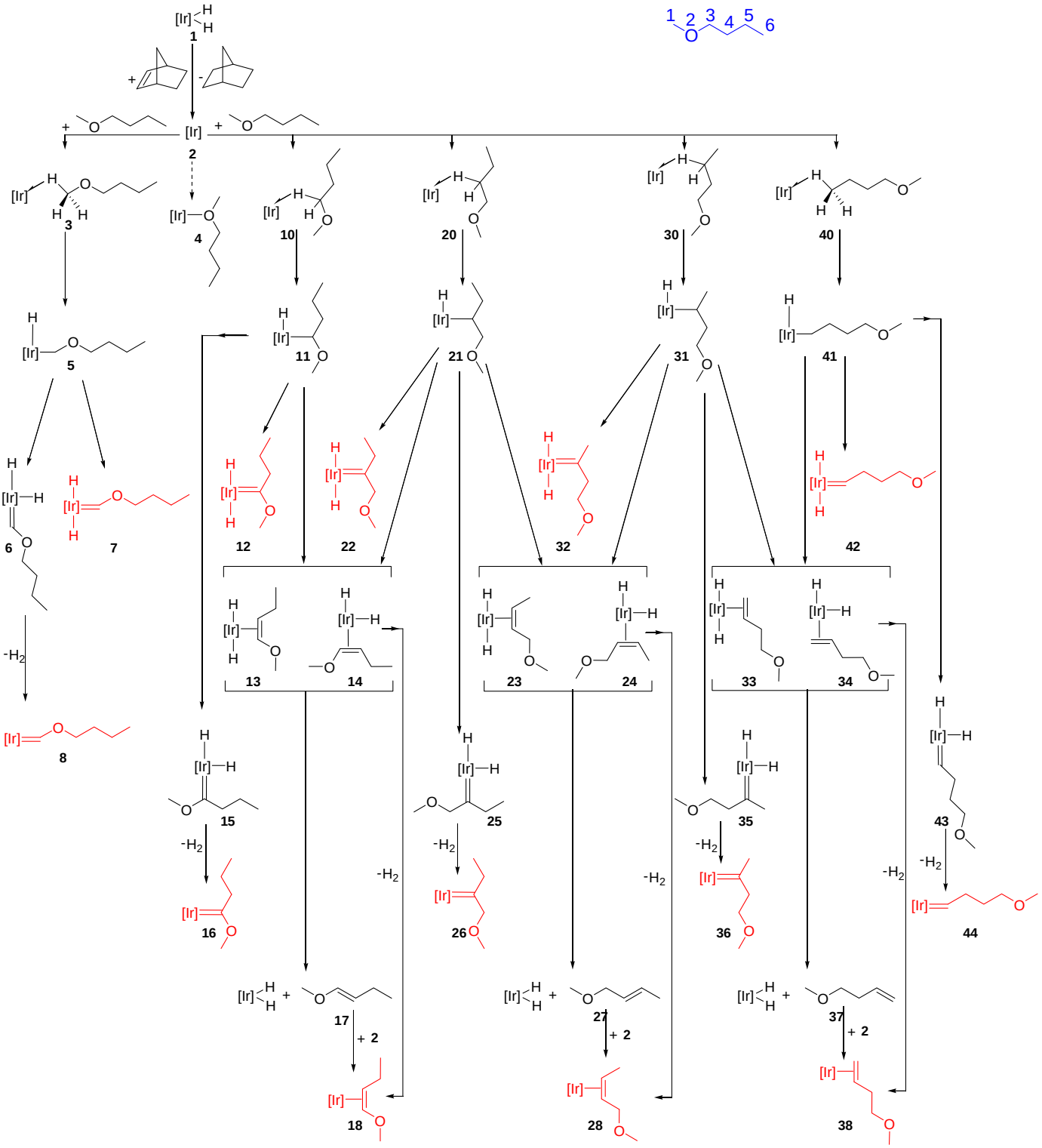
2. n-Butyl Methyl Ether (NBE)

2.1. Experimental reaction of (PNP)IrH$_2$ (1) with Norbornylene in *n*-Butyl Methyl Ether

(PNP)IrH$_2$ (**1**) and nobornylene (3 equiv) were combined in NBE (700 µL), and the resulting brown solution was transferred to a J. Young tube. ^{31}P NMR spectroscopy after 10 min revealed quantitative formation of a single intermediate species (δ 45.4 ppm). The solution was frozen and the headspace evacuated and backfilled with carbon monoxide (1 atm). As the solution thawed, an immediate color change from brown to yellow was observed, and ^{31}P NMR revealed a mixture containing a new species (δ 30.8 ppm) along with small amounts of (PNP)Ir–CO (δ 57.6 ppm, 4%) and an unidentified side product (δ 26.5 ppm, 2%). ^{1}H NMR (C_6D_6) δ 7.72 (dt, J_1 = 8.3 Hz, J_2 = 2.3 Hz, 2H, Ar–*H*), 6.93 (m, 2H, Ar–*H*), 6.75 (dd, J_1 = 8.6 Hz, J_2 = 1.8 Hz, 2H, Ar–*H*), 4.58 (t, $^{3}J_{PH}$ = 4.5 Hz, 2H,–C*H*$_2$O^{n}Bu), 3.40 (t, *J* = 6 Hz, 2H, –OC*H*$_2^{n}$Pr), 2.51 (m, 2H, –C*H*(CH$_3$)$_2$), 2.21 (s, 6H, Ar–C*H*$_3$), 2.20 (m, 2H, –C*H*(CH$_3$)$_2$), 1.69–1.11 (m, 28H, –CH(C*H*$_3$)$_2$ and –OCH$_2$C*H*$_2$C*H*$_2$CH$_3$), 0.85 (t, $^{3}J_{HH}$ = 7.3 Hz, 3H, –O(CH$_2$)$_3$C*H*$_3$), –8.15 (t, $^{2}J_{PH}$ = 18 Hz, 1H, Ir–*H*). IR (C_6D_6, KBr, cm^{-1}) ν(CO): 1976 cm^{-1}.

2.2. n-Butyl methyl ether (NBE) relative energy diagrams and tables.

Scheme S2



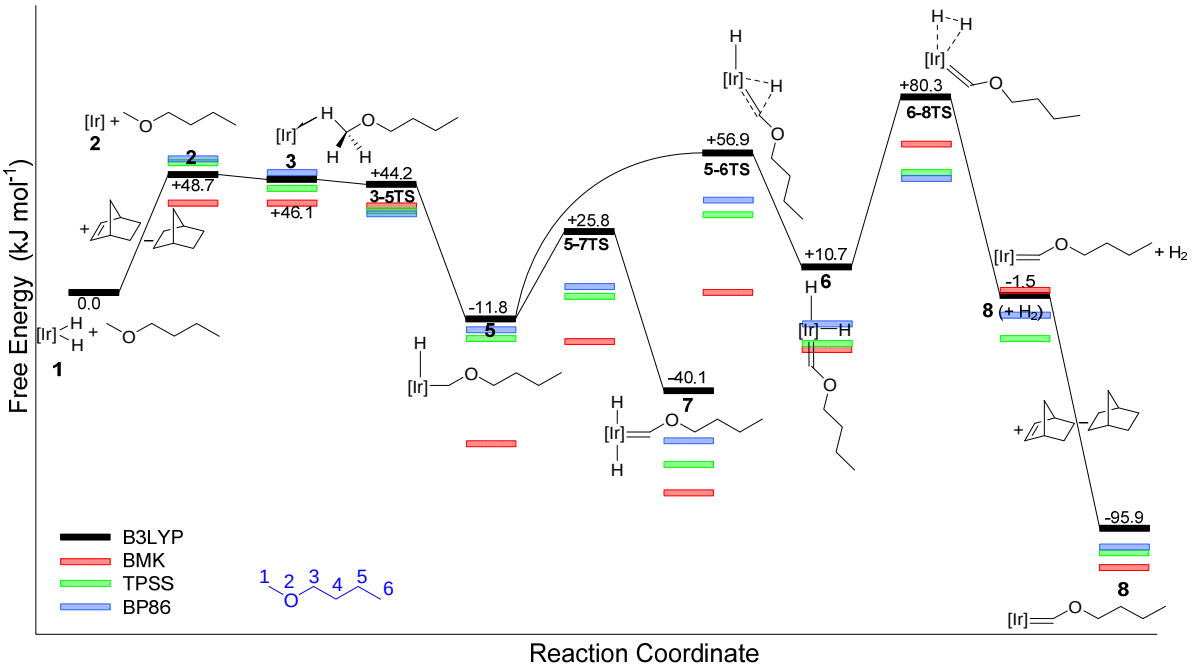


Figure S12 Relative energy surface for the formation of carbene $\mathbf{8}_{\mathbf{NBE}}$. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

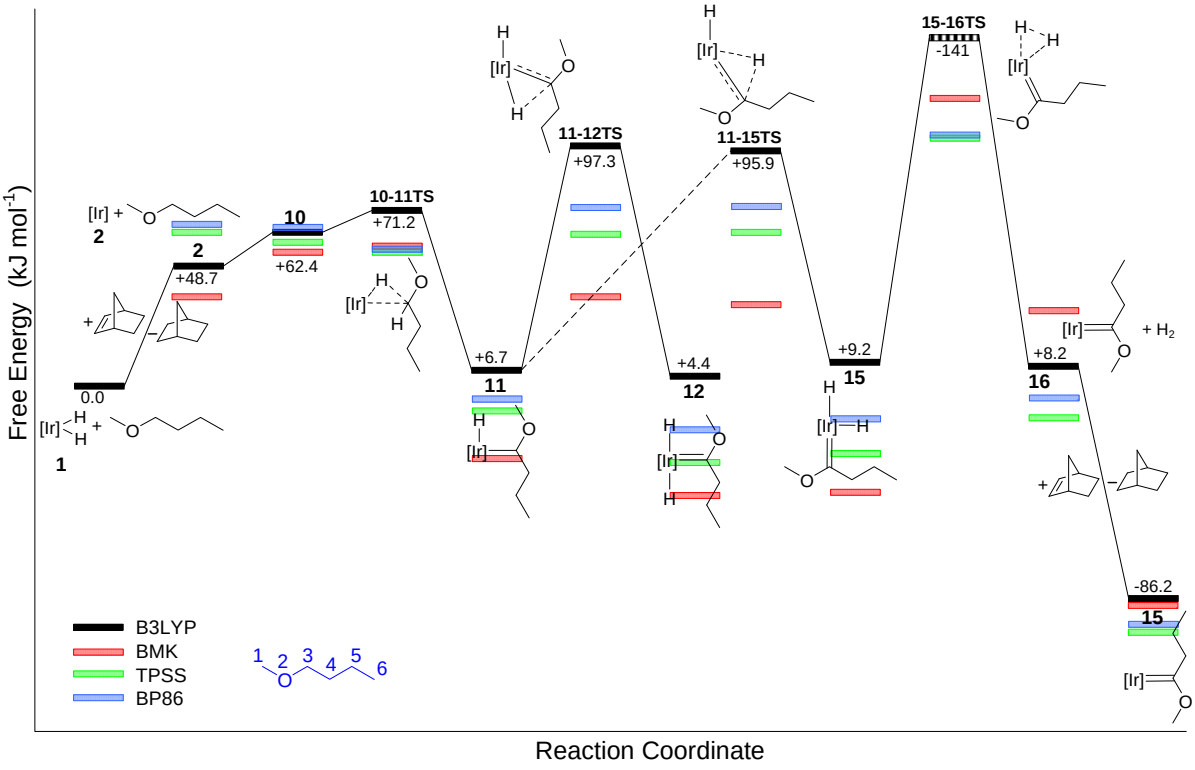


Figure S13. Relative energy surface for the formation of carbene **15**$_{NBE}$. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}. Note **15-16TS**$_{NBE}$ is not a converged structure.

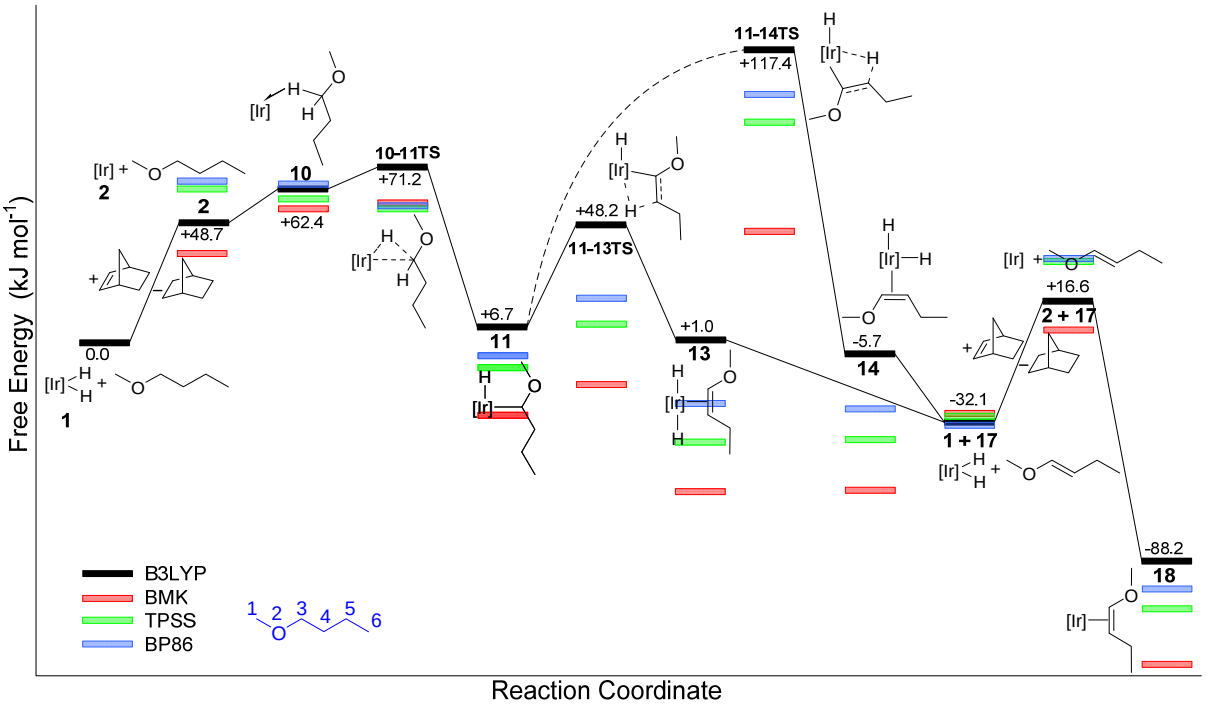


Figure S14. Relative energy surface for the formation of vinyl ether adduct 1**8**$_{NBE}$. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

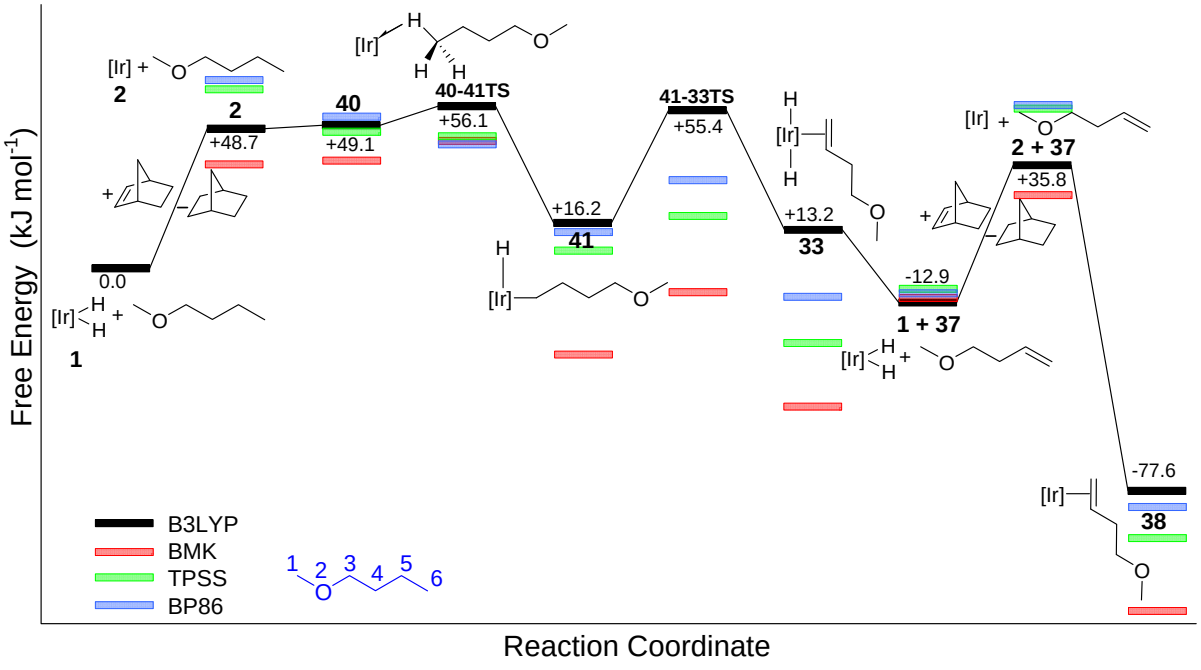


Figure S15. Relative energy surface for the formation of vinyl ether adduct 3**8**$_{NBE}$. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

Table S1. Energy (in kJ mol^{-1}) of selected *n*-butyl ether vinyl ether intermediates and products. Structure numbers in **bold**.

Ir-(C-C) bond	Trans-dihydrido vinyl ethyl intermediate. Model-opt	Vinyl ether adduct. Model-opt	Vinyl ether adduct. Full-opt
C3-C4	**13** = +1.8	**18** = -88.2	**18** = -30.5
C4-C5	**23** = +13.8	**28** = -77.3	-
C5-C6	**33** = +13.2	**38** = -77.6	**38** = -29.6

2.3. Intermediates in the reactions of NBE with (PNP)IrH_2 (1)

As a final point on the NBE reaction, the experimental CO intermediate trapping experiments indicated the presence, almost exclusively, of methyl intermediate $\mathbf{5_{NBE}}$, but a small amount of another, not identifiable C-H activated intermediate was also observed.[2] It might well be assumed that this intermediate is from the other lowest energy competing pathway to vinyl ether formation, that being from $\mathbf{11_{NBE}}$ (see Figure 7 manuscript). It is certainly low enough in energy to suggest that its presence may be observed. However when consideration is given to every C-H activation position along the *n*-butyl ether chain we see an interesting trend, which is perhaps best outlined in Table S2.

Table S2. Energy (in kJ mol^{-1}) of selected *n*-butyl ether carbene intermediates and products at the Model opt level of theory. Structure numbers in **bold**.

Ir-C bond	Agostic C-H	C-H Transition Structure	C-H activation Product	Carbene Product*
C1	**3** = +48.6	**3-5TS** = +44.2	**5** = -11.8	**8** = -95.9
C3	**10** = +62.4	**10-11TS** = +71.2	**11** = +6.7	**16** = -86.2
C4	**20** = +74.5	**20-21TS** = +87.3	**21** = +7.7	**26** = +2.3
C5	**30** = +68.6	**30-31TS** = +86.4	**31** = +28.0	**36** = -5.2
C6	**40** = +49.1	**40-41TS** = +56.1	**41** = +16.2	**44** = -11.9

* Energy calculated after indirect interaction of H_2 with excess norbornylene.

Notice the structure energies resulting from coordination at the C6 position (the opposite end of the molecule). The transition barriers at $\mathbf{40_{NBE}}$ and $\mathbf{40\text{-}41TS_{NBE}}$ (see Scheme S2)are quite low being +49.1 and +56.1 kJ mol^{-1} respectively, suggesting that an intermediate from this path ($\mathbf{41_{NBE}}$) may be the next most likely intermediate observed. Since we have shown that steric influence governs initial binding it is really no surprise to find the next lowest energy barrier to be from a terminal methyl group, so perhaps this C6 C-H activated intermediate ($\mathbf{41_{NBE}}$) is this unidentified intermediate, not from the expected C3 methylene position. One other aspect of Table S2 worth noting is the energy of the carbene end products in the column to the right. The stable carbenes $\mathbf{8_{NBE}}$ and $\mathbf{16_{NBE}}$ both have the etheral oxygen adjacent to the Ir-C bond in support of our discussion earlier for the DEE reactions where we stated “Carbenes will only form at the carbon directly adjacent to the oxygen.”

2.4. Coordinates of NBE structures at the Model-opt level of theory

Structure n-butyl ether (NBE)
B3LYP/GBS(1) = -272.967302a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -273.061615 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -272.861417 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -273.095835 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -273.04498037 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -272.847885 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -272.268553 a.u.
Enthalpy Correction = 0.175415
Gibbs Free Energy Correction = 0.134156

Atomic No	x-coord	y-coord	z-coord
6	-2.785416	-0.465423	0.025334
1	-3.176240	-1.370438	-0.448022
1	-2.916567	-0.548911	1.117075
1	-3.371299	0.400977	-0.324566
8	-1.427241	-0.357752	-0.332543
6	-0.800561	0.786137	0.220122
6	0.664462	0.800731	-0.201116
1	-0.883195	0.768582	1.322134
1	-1.309774	1.701846	-0.128667
6	1.470069	-0.391210	0.331717
1	0.710335	0.819125	-1.298532
1	1.111799	1.741924	0.149141
6	2.934328	-0.370876	-0.117832
1	1.422966	-0.394624	1.430553
1	0.989027	-1.318486	-0.000132
1	3.485443	-1.231524	0.278366
1	3.013293	-0.400566	-1.211666
1	3.444848	0.537960	0.225309

Structure 3 - NBE
B3LYP/GBS(1) = -1429.643071 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.946266 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.701308 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.014447 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.057351 a.u.
Enthalpy Correction = 0.420513
Gibbs Free Energy Correction = 0.337467

Atomic No	x-coord	y-coord	z-coord
7	2.416695	1.222390	-0.259815
6	3.675568	0.696034	-0.376746

6	3.926623	-0.638541	-0.290321
1	4.480488	1.415006	-0.542491
1	4.933672	-1.031856	-0.386477
6	2.234562	2.580517	-0.323695
6	1.016071	3.169529	-0.188788
1	3.136108	3.173835	-0.489645
1	0.901870	4.247440	-0.245945
15	2.468376	-1.639935	-0.007255
15	-0.329756	2.013534	0.071213
8	-2.441370	-0.785746	0.485400
6	-3.543558	-1.364527	-0.201002
1	-3.629758	-2.433145	0.061851
1	-3.379964	-1.310332	-1.291203
6	2.810724	-2.674315	1.494815
1	1.984365	-3.372130	1.671556
1	3.737457	-3.248726	1.379623
1	2.901723	-2.016014	2.362834
6	2.449144	-2.942322	-1.330477
1	3.381843	-3.518552	-1.335827
1	1.611958	-3.631123	-1.169766
1	2.321601	-2.459081	-2.302915
6	-1.238848	2.531748	1.598108
1	-1.611115	3.559619	1.514320
1	-2.082867	1.853015	1.756865
1	-0.564728	2.461429	2.455882
6	-1.599715	2.350077	-1.235642
1	-2.449302	1.675613	-1.088707
1	-1.952630	3.387312	-1.195625
1	-1.161138	2.157620	-2.218522
77	0.828070	0.005354	0.056931
6	-1.225309	-1.439015	0.193234
1	-0.463002	-0.997621	0.943745
1	-1.249385	-2.500462	0.484172
1	-0.957678	-1.374343	-0.872477
6	-4.814404	-0.620836	0.189315
1	-4.921715	-0.661614	1.281236
1	-4.700122	0.439005	-0.075452
6	-6.068248	-1.194529	-0.483845
1	-6.173514	-2.255372	-0.215952
1	-5.943186	-1.166108	-1.575550
6	-7.347011	-0.443312	-0.098338
1	-8.225718	-0.874289	-0.591174
1	-7.518025	-0.482630	0.984315
1	-7.287419	0.613429	-0.385942

Structure 3-5TS - NBE

B3LYP/GBS(1) = -1429.641223 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.946728 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.701500 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.018384 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.063063 a.u.
Enthalpy Correction = 0.416935
Gibbs Free Energy Correction = 0.336250
Imaginary Freq = -642.0i

Atomic No	x-coord	y-coord	z-coord
7	-2.309638	1.255308	-0.313250
6	-3.556548	0.728111	-0.519279
6	-3.804894	-0.609506	-0.481137
1	-4.357377	1.443281	-0.723080
1	-4.802608	-1.004209	-0.645927
6	-2.105359	2.608273	-0.406373
6	-0.880334	3.179943	-0.256147
1	-2.988989	3.216729	-0.614655
1	-0.746837	4.254413	-0.335069
15	-2.364143	-1.623199	-0.137880
15	0.450451	2.018029	0.070426
8	2.250717	-0.777855	1.126787
6	3.065205	-1.284124	0.079910
1	2.652204	-0.973836	-0.895632
1	3.058039	-2.387645	0.100741
6	-2.238370	-2.870095	-1.503217
1	-1.419093	-3.568442	-1.299299
1	-3.169422	-3.438882	-1.609894
1	-2.026030	-2.348492	-2.440004
6	-2.814643	-2.710054	1.297425
1	-3.716637	-3.296346	1.086215
1	-1.992892	-3.399105	1.523392
1	-2.994625	-2.082524	2.174634
6	1.758143	2.333975	-1.202962
1	2.061453	3.387436	-1.203033
1	2.636272	1.713729	-0.995826
1	1.366954	2.072659	-2.189660
6	1.303462	2.571405	1.617105
1	2.105360	1.863081	1.847123
1	1.720745	3.579553	1.510680
1	0.584030	2.566772	2.440707
77	-0.718023	0.007659	0.073872
6	0.922684	-1.243231	1.088693
1	0.562073	-0.998403	-0.229021
1	0.892074	-2.339067	1.001591
1	0.450032	-0.949833	2.029018
6	4.485556	-0.761811	0.255924
1	4.464296	0.336580	0.247514
1	4.847811	-1.058790	1.248957
6	5.444067	-1.272393	-0.828068
1	5.066342	-0.979452	-1.817861
1	5.453596	-2.371494	-0.818447
6	6.873909	-0.749566	-0.653537
1	7.535810	-1.130261	-1.439549
1	6.902888	0.346174	-0.694549
1	7.292124	-1.055666	0.313053

Structure 4 – NBE (ether bound by oxygen)

B3LYP/GBS(1) = -1429.657641 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.954041 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.714332 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.022960 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.062288 a.u.
Enthalpy Correction = 0.421861
Gibbs Free Energy Correction = 0.338892

Atomic No	x-coord	y-coord	z-coord
7	1.925189	0.809427	-1.000031
6	1.970437	2.125460	-1.370218
6	1.018112	3.023300	-0.995015
1	2.819337	2.423791	-1.989264
1	1.069322	4.064116	-1.299738
6	2.926573	-0.035350	-1.395034
6	2.957549	-1.352847	-1.049243
1	3.713352	0.406371	-2.010510
1	3.761958	-2.004152	-1.376781
15	-0.286966	2.328297	0.016756
15	1.575314	-1.870394	-0.036735
8	-1.182607	-0.753192	1.471258
6	-1.879229	2.814209	-0.817052
1	-2.741513	2.510661	-0.211872
1	-1.928475	3.898519	-0.973801
1	-1.938771	2.313177	-1.787111
6	-0.387197	3.394743	1.538553
1	-0.479328	4.455360	1.275417
1	-1.253241	3.112507	2.149012
1	0.519886	3.251743	2.132032
6	0.817134	-3.345032	-0.875864
1	1.558526	-4.136907	-1.036707
1	0.000608	-3.747222	-0.265434
1	0.410906	-3.034463	-1.842245
6	2.286734	-2.686449	1.475104
1	1.481203	-3.093774	2.097047
1	2.967848	-3.502991	1.207049
1	2.835468	-1.940453	2.056514
77	0.403869	0.116478	0.156901
6	-2.567027	-0.689053	1.079688
6	-2.748913	-1.255484	-0.319373
1	-2.902459	0.357702	1.130575
1	-3.145606	-1.267145	1.814788
1	-2.067341	-0.720172	-0.993804
1	-2.433235	-2.307091	-0.320771
6	-0.990805	-0.460776	2.858600
1	-1.568025	-1.171757	3.465119
1	-1.306801	0.564230	3.091628
6	-4.201155	-1.141616	-0.804381
1	-4.871538	-1.655839	-0.100244
1	-4.505545	-0.085366	-0.801182
6	-4.397595	-1.721985	-2.209163
1	-5.438263	-1.624429	-2.538334
1	-3.763982	-1.206150	-2.940346
1	-4.136272	-2.786747	-2.237187
1	0.075649	-0.565981	3.055028

Structure 5 - NBE

B3LYP/GBS(1) = -1429.662082 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.966541 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.737387 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.037272 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.079796 a.u.

Enthalpy Correction = 0.416981
Gibbs Free Energy Correction = 0.334729

Atomic No	x-coord	y-coord	z-coord
7	-2.479860	1.230447	-0.012314
6	-3.703947	0.642502	0.061046
6	-3.867836	-0.714735	0.097097
1	-4.575973	1.303571	0.093688
1	-4.858659	-1.156205	0.150133
6	-2.317100	2.583755	0.028339
6	-1.086443	3.175860	0.034123
1	-3.225214	3.194181	0.059728
1	-0.989790	4.257193	0.063401
15	-2.365210	-1.697111	0.053390
15	0.328632	2.064561	0.000810
8	2.207989	-0.521575	0.006066
6	3.340147	-1.343833	-0.188735
1	3.367280	-1.720189	-1.228613
1	3.285028	-2.232127	0.466826
6	-2.543778	-2.902856	-1.343853
1	-1.675841	-3.570456	-1.374909
1	-3.452225	-3.505889	-1.232051
1	-2.598813	-2.356395	-2.289945
6	-2.380776	-2.824606	1.519103
1	-3.282186	-3.447769	1.532012
1	-1.497675	-3.472272	1.498223
1	-2.348999	-2.221680	2.430369
6	1.389921	2.535739	-1.437963
1	1.736435	3.572281	-1.356196
1	2.249037	1.859116	-1.462897
1	0.820368	2.425268	-2.365577
6	1.417971	2.458949	1.435438
1	2.256654	1.757885	1.424819
1	1.788339	3.489114	1.385584
1	0.852738	2.324204	2.361476
6	0.964165	-1.205008	-0.239975
1	0.945168	-2.109672	0.394983
1	0.984671	-1.577956	-1.291470
77	-0.721989	-0.019169	-0.048785
1	-0.602697	-0.062233	1.496759
6	4.605662	-0.547699	0.114068
1	4.625400	0.342027	-0.530880
1	4.552468	-0.182797	1.149094
6	5.891292	-1.360275	-0.085437
1	5.861990	-2.253254	0.555057
1	5.932766	-1.729342	-1.120123
6	7.160846	-0.557742	0.219293
1	8.062588	-1.162418	0.068641
1	7.237506	0.323213	-0.429993
1	7.165839	-0.203944	1.257667

Structure 5-6TS - NBE
B3LYP/GBS(1) = -1429.626827 a.u.

B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.938892 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.712321 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.016212 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.058370 a.u.
Enthalpy Correction = 0.413586
Gibbs Free Energy Correction = 0.333246
Imaginary Freq = -102.2 i

Atomic No	x-coord	y-coord	z-coord
7	-2.360049	0.948534	-0.666218
6	-3.453518	0.210445	-1.006600
6	-3.546248	-1.128218	-0.773429
1	-4.266927	0.756065	-1.488765
1	-4.430941	-1.688327	-1.059277
6	-2.329727	2.296438	-0.884343
6	-1.265330	3.072021	-0.548710
1	-3.217535	2.723791	-1.354267
1	-1.264209	4.139372	-0.746815
15	-2.128926	-1.862412	0.031841
15	0.128569	2.199996	0.166048
8	2.218778	-0.399335	-0.371984
6	3.312621	-1.204412	0.065279
1	3.240495	-2.206501	-0.388035
1	3.262061	-1.334579	1.159666
6	-1.614618	-3.322695	-0.984208
1	-0.787537	-3.853994	-0.499982
1	-2.448019	-4.021913	-1.117764
1	-1.278304	-2.968044	-1.961712
6	-2.714635	-2.685032	1.583004
1	-3.509192	-3.410229	1.372329
1	-1.882144	-3.203855	2.071036
1	-3.093979	-1.917784	2.262259
6	1.597681	2.650968	-0.860189
1	1.718405	3.740060	-0.899220
1	2.497593	2.191827	-0.445241
1	1.452345	2.263277	-1.871415
6	0.542993	3.004727	1.779338
1	1.430518	2.530269	2.211716
1	0.742148	4.074572	1.647932
1	-0.295893	2.871858	2.466640
6	0.961426	-0.957518	-0.205865
1	1.013083	-2.049157	-0.325282
77	-0.745446	0.023399	0.225355
1	0.654466	-0.863999	1.035492
1	-1.630075	0.495329	1.526456
6	4.617714	-0.528515	-0.335713
1	4.654200	0.469738	0.121415
1	4.612238	-0.375757	-1.423005
6	5.857570	-1.333019	0.076187
1	5.814086	-2.331220	-0.382094
1	5.844109	-1.495503	1.163300
6	7.170204	-0.648181	-0.319513
1	7.259720	0.338203	0.151846
1	8.038375	-1.243563	-0.014900
1	7.228949	-0.502529	-1.405021

Structure 5-7TS - NBE

B3LYP/GBS(1) = -1429.639784 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.949324 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.718679 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.027951 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.069717 a.u.
Enthalpy Correction = 0.412386
Gibbs Free Energy Correction = 0.331821
Imaginary Freq = -808.2 i

Atomic No	x-coord	y-coord	z-coord
77	0.688652	-0.006742	0.130807
7	2.503688	0.965581	-0.514086
6	2.507290	2.316769	-0.651950
6	1.405309	3.082533	-0.402781
1	3.445167	2.780519	-0.972590
1	1.434905	4.161195	-0.525416
6	3.615033	0.214158	-0.710404
6	3.636338	-1.136955	-0.505156
1	4.517222	0.737432	-1.041929
1	4.542048	-1.713920	-0.666541
15	-0.071465	2.206128	0.120508
15	2.111138	-1.872657	0.079014
8	-2.228441	-0.370094	0.090865
6	-3.336845	-1.123960	-0.430489
1	-3.243568	-2.172692	-0.114018
1	-3.296246	-1.095397	-1.528726
6	-1.002014	-0.930271	0.027805
1	-1.087947	-2.016314	-0.128471
6	-1.428940	2.703100	-1.033777
1	-2.356721	2.205169	-0.737197
1	-1.577745	3.789184	-1.026383
1	-1.165528	2.383198	-2.045433
6	-0.645399	2.956097	1.709218
1	-0.809688	4.034725	1.603292
1	-1.580614	2.479608	2.021457
1	0.111617	2.777468	2.476572
6	1.719639	-3.295314	-1.042389
1	2.549175	-4.010725	-1.081016
1	0.823988	-3.820314	-0.690078
1	1.529414	-2.912304	-2.048448
6	2.486394	-2.757479	1.660722
1	1.597431	-3.291868	2.013256
1	3.304318	-3.475296	1.528979
1	2.770491	-2.019400	2.414648
1	1.347374	0.349773	1.574489
1	-0.234225	-0.533450	-1.331624
6	-4.630171	-0.510162	0.085926
1	-4.664778	0.545999	-0.212763
1	-4.613354	-0.525991	1.183573
6	-5.877930	-1.238125	-0.432210
1	-5.833234	-2.296086	-0.137311
1	-5.878333	-1.226687	-1.531242
6	-7.181526	-0.620043	0.084411
1	-7.272993	0.427918	-0.225858
1	-8.055581	-1.158806	-0.297957

1	-7.225261	-0.646295	1.179919

Structure 6 - NBE

B3LYP/GBS(1) = -1429.649086 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.957238 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.721974 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.037879 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.078537 a.u.
Enthalpy Correction = 0.414684
Gibbs Free Energy Correction = 0.333981

Atomic No	x-coord	y-coord	z-coord
7	0.920331	0.308756	1.739680
6	1.555979	-0.690873	2.404727
6	2.096431	-1.773944	1.772492
1	1.628004	-0.591748	3.492266
1	2.592378	-2.558652	2.336431
6	0.519613	1.454728	2.355877
6	0.019214	2.521482	1.670892
1	0.624096	1.490825	3.444574
1	-0.303203	3.418130	2.192486
15	1.986824	-1.782841	-0.020176
15	-0.040210	2.364663	-0.120560
8	-2.107711	-0.206148	-1.016107
6	-3.170063	-1.029246	-1.558031
1	-2.730701	-1.766451	-2.241116
1	-3.796807	-0.344314	-2.137724
6	1.309363	-3.443183	-0.496248
1	1.284920	-3.546697	-1.586699
1	1.930450	-4.245462	-0.082091
1	0.293562	-3.554388	-0.106300
6	3.704266	-1.903205	-0.690530
1	4.228918	-2.777836	-0.288602
1	3.670405	-1.973968	-1.782911
1	4.243936	-0.993561	-0.418179
6	-1.741373	2.884257	-0.631763
1	-1.961623	3.893324	-0.264079
1	-1.818196	2.878612	-1.724174
1	-2.469844	2.178512	-0.230128
6	0.970153	3.741315	-0.828928
1	0.920150	3.707645	-1.922473
1	0.611172	4.717481	-0.482177
1	2.009469	3.600925	-0.524627
6	-0.893900	-0.723977	-0.855452
1	-0.905202	-1.775956	-1.197740
77	0.781811	0.189693	-0.399838
1	1.049651	0.289248	-1.999715
1	2.286902	0.935628	-0.389710
6	-3.968279	-1.706331	-0.449028
1	-3.300605	-2.380077	0.106444
1	-4.725223	-2.344412	-0.928106
6	-4.647515	-0.730273	0.520132

1	-3.883992	-0.091706	0.980401
1	-5.311043	-0.061784	-0.047057
6	-5.449866	-1.444195	1.612762
1	-4.805303	-2.095464	2.215612
1	-5.922275	-0.724930	2.290893
1	-6.243418	-2.068046	1.182750

Structure 6-8TS - NBE

B3LYP/GBS(1) = -1429.615397 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.926757 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.685793 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.006180 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.050828 a.u.
Enthalpy Correction = 0.410795
Gibbs Free Energy Correction = 0.330028
Imaginary Freq = -752.1 i

Atomic No	x-coord	y-coord	z-coord
7	-2.255903	0.864920	-0.978539
6	-3.240025	0.048762	-1.429929
6	-3.328793	-1.267000	-1.073706
1	-3.979047	0.489543	-2.106622
1	-4.131984	-1.894943	-1.448199
6	-2.164878	2.169534	-1.346406
6	-1.159596	2.982521	-0.914066
1	-2.941663	2.551675	-2.016252
1	-1.107864	4.021974	-1.225448
15	-2.060134	-1.880760	0.035285
15	0.081664	2.234180	0.150441
8	2.163488	-0.358446	0.012883
6	3.241412	-1.251849	-0.309885
1	3.143087	-1.573121	-1.356723
1	3.176049	-2.145538	0.326977
6	-1.354499	-3.404876	-0.748737
1	-0.637828	-3.888121	-0.075354
1	-2.150491	-4.120720	-0.982339
1	-0.841267	-3.129613	-1.674032
6	-2.921373	-2.611693	1.503322
1	-3.666885	-3.354583	1.196762
1	-2.192747	-3.090628	2.166356
1	-3.421022	-1.809839	2.053450
6	1.714989	2.621305	-0.625193
1	1.794188	3.697092	-0.820624
1	2.528268	2.307156	0.033733
1	1.801057	2.074319	-1.566832
6	0.169010	3.264096	1.687505
1	0.969639	2.893790	2.336678
1	0.361443	4.316599	1.448825
1	-0.781229	3.186725	2.222422
6	0.911844	-0.875405	0.040966
1	0.973036	-1.965121	-0.114712
77	-0.736630	0.038620	0.348753
1	-1.031622	0.181114	2.010801
1	-1.884514	0.587532	1.646996
6	4.560563	-0.525088	-0.089093

1	4.573315	0.380121	-0.710381
1	4.607261	-0.190922	0.955883
6	5.778878	-1.399060	-0.415422
1	5.715545	-1.740298	-1.458376
1	5.755178	-2.306244	0.204886
6	7.108503	-0.668708	-0.198543
1	7.960850	-1.314763	-0.436797
1	7.177751	0.223537	-0.832604
1	7.216226	-0.343873	0.843448

Structure 7 - NBE

B3LYP/GBS(1) = -1429.657697 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.966132 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.730480 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.045366 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.086351 a.u.
Enthalpy Correction = 0.413711
Gibbs Free Energy Correction = 0.331948

Atomic No	x-coord	y-coord	z-coord
77	0.675221	-0.011656	0.000078
7	2.555265	1.050575	-0.000479
6	2.533059	2.408795	-0.000575
6	1.372349	3.125631	-0.000333
1	3.500505	2.920148	-0.000865
1	1.385899	4.211518	-0.000416
6	3.711707	0.342871	-0.000724
6	3.737739	-1.022345	-0.000627
1	4.644895	0.914471	-0.001010
1	4.677382	-1.566454	-0.000824
15	-0.152422	2.178300	0.000145
15	2.146535	-1.845533	-0.000149
8	-2.190404	-0.434581	0.001091
6	-3.327302	-1.329996	0.001525
1	-3.274626	-1.967427	0.893311
1	-3.273499	-1.969865	-0.888444
6	-0.965629	-0.965213	0.000474
1	-1.033822	-2.067458	0.000139
6	-1.165752	2.760334	-1.431833
1	-2.127240	2.236717	-1.433936
1	-1.344781	3.840719	-1.381555
1	-0.633377	2.521543	-2.355512
6	-1.164986	2.760463	1.432610
1	-1.344249	3.840805	1.382232
1	-2.126367	2.236654	1.435388
1	-0.632015	2.521944	2.356014
6	2.130515	-3.019760	-1.431551
1	2.972838	-3.719840	-1.383979
1	1.197048	-3.594183	-1.439479
1	2.190580	-2.440531	-2.356000

6	2.131249	-3.019506	1.431470
1	1.197790	-3.593930	1.439974
1	2.973556	-3.719585	1.383597
1	2.191777	-2.440110	2.355784
1	0.814232	0.088162	1.672780
1	0.813499	0.087801	-1.672712
6	-4.594925	-0.490196	-0.000373
1	-4.584309	0.165920	0.879816
1	-4.583215	0.163649	-0.882237
6	-5.868720	-1.346589	-0.000040
1	-5.865832	-2.007355	-0.878271
1	-5.866638	-2.005473	0.879610
6	-7.147161	-0.501613	-0.001528
1	-8.041156	-1.134804	-0.001337
1	-7.194973	0.145039	0.882889
1	-7.194095	0.143267	-0.887286

Structure 8 - NBE

B3LYP/GBS(1) = -1428.464215 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1428.761381 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1427.523985 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1428.836070 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1428.879327 a.u.
Enthalpy Correction = 0.397354
Gibbs Free Energy Correction = 0.314387

Atomic No	x-coord	y-coord	z-coord
77	-0.690899	-0.006983	-0.000034
7	-2.522341	1.052499	0.000097
6	-2.500004	2.423980	0.000095
6	-1.340791	3.137749	0.000044
1	-3.468182	2.934050	0.000145
1	-1.351606	4.223677	0.000047
6	-3.704103	0.360904	0.000161
6	-3.753347	-1.000251	0.000164
1	-4.625433	0.951470	0.000203
1	-4.701357	-1.529720	0.000211
15	0.171556	2.155558	-0.000032
15	-2.154799	-1.827891	0.000095
8	2.178791	-0.425636	-0.000330
6	3.304974	-1.323877	-0.000698
1	3.253222	-1.965577	-0.890831
1	3.252711	-1.966967	0.888401
6	0.936675	-0.963570	-0.000287
1	1.030449	-2.065675	-0.000474
6	1.184889	2.734949	1.435683
1	2.132183	2.186892	1.448401
1	1.387847	3.810589	1.376466
1	0.644287	2.521059	2.361541
6	1.184786	2.735018	-1.435793
1	1.387727	3.810659	-1.376553
1	2.132087	2.186975	-1.448583

1	0.644131	2.521146	-2.361624
6	-2.171429	-3.004850	1.433236
1	-3.026940	-3.688159	1.379234
1	-1.248630	-3.595401	1.445610
1	-2.228314	-2.430690	2.361820
6	-2.171606	-3.004964	-1.432950
1	-1.248794	-3.595494	-1.445409
1	-3.027092	-3.688290	-1.378770
1	-2.228638	-2.430881	-2.361573
6	4.582770	-0.497810	0.000303
1	4.578974	0.158645	-0.879946
1	4.578629	0.157075	0.881719
6	5.848124	-1.366245	-0.000228
1	5.838464	-2.027150	0.877959
1	5.838743	-2.025670	-0.879531
6	7.136341	-0.536277	0.000680
1	8.023559	-1.179195	0.000236
1	7.191212	0.109954	-0.883739
1	7.190974	0.108399	0.886249

Structure 10 - NBE

B3LYP/GBS(1) = -1429.641564 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.941335 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.696090 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.010638 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.052625 a.u.
Enthalpy Correction = 0.420703
Gibbs Free Energy Correction = 0.337768

Atomic No	x-coord	y-coord	z-coord
7	-2.351701	0.090076	-0.511031
6	-3.091989	-1.059650	-0.598765
6	-2.574685	-2.291068	-0.341089
1	-4.136337	-0.932291	-0.890957
1	-3.183200	-3.186498	-0.419453
6	-2.931236	1.301079	-0.787425
6	-2.250924	2.477205	-0.723710
1	-3.986021	1.269766	-1.067903
1	-2.735213	3.421962	-0.949637
15	-0.841560	-2.275906	0.114541
15	-0.531151	2.300478	-0.250164
8	2.430352	0.808167	1.932046
6	0.017576	-3.453561	-1.035348
1	1.075482	-3.545100	-0.765146
1	-0.441529	-4.448617	-0.999855
1	-0.048656	-3.064208	-2.054717
6	-0.706370	-3.202675	1.718242
1	-1.145710	-4.203788	1.635781
1	0.344983	-3.306303	2.010329
1	-1.231831	-2.644307	2.497606
6	0.479941	3.135334	-1.563327
1	0.167585	4.176957	-1.702943

1	1.539782	3.120840	-1.285739
1	0.357159	2.594116	-2.505193
6	-0.234866	3.434994	1.186744
1	0.814396	3.369300	1.494433
1	-0.469487	4.474724	0.930061
1	-0.865358	3.122221	2.023475
77	-0.399335	0.000806	0.018557
6	2.340765	-0.104278	0.882781
6	3.552082	0.037296	-0.034386
1	1.454185	0.140931	0.187144
1	2.228681	-1.133695	1.245754
1	3.620618	1.085273	-0.353881
1	4.451476	-0.171255	0.560363
6	1.505421	0.556634	2.981631
1	1.721928	-0.403055	3.475623
1	0.477317	0.532577	2.584239
6	3.491007	-0.885006	-1.257280
1	3.441492	-1.931301	-0.923069
1	2.558323	-0.693217	-1.804593
6	4.690973	-0.706607	-2.193471
1	4.621302	-1.375720	-3.058293
1	4.747940	0.321459	-2.571427
1	5.635018	-0.923102	-1.678395
1	1.618014	1.367663	3.705098

Structure 10-11TS - NBE

B3LYP/GBS(1) = -1429.631923 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.936180 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.693290 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.010471 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.054348 a.u.
Enthalpy Correction = 0.416396
Gibbs Free Energy Correction = 0.335993
Imaginary Freq = -712.1 i

Atomic No	x-coord	y-coord	z-coord
7	1.752121	1.586409	-0.141584
6	1.449332	2.920977	-0.065796
6	0.177069	3.379613	0.079952
1	2.291815	3.614098	-0.133769
1	-0.037753	4.442210	0.136327
6	3.040968	1.184480	-0.388746
6	3.384571	-0.119490	-0.559684
1	3.791198	1.976938	-0.450755
1	4.412627	-0.410714	-0.751945
15	-1.078603	2.096282	0.120314
15	2.014711	-1.277967	-0.441252
8	-0.655119	-2.269993	1.566073
6	-2.271644	2.495646	-1.241478
1	-3.115737	1.798953	-1.221771
1	-2.652174	3.518913	-1.142418
1	-1.758518	2.395145	-2.201457

6	-2.122282	2.431085	1.618522
1	-2.536952	3.445538	1.597408
1	-2.950988	1.715407	1.669493
1	-1.506518	2.316055	2.514982
6	1.966150	-2.220142	-2.036948
1	2.935905	-2.683195	-2.253000
1	1.203371	-3.004309	-1.982262
1	1.704836	-1.534692	-2.847266
6	2.558153	-2.605738	0.730905
1	1.756525	-3.341785	0.841536
1	3.465562	-3.101886	0.367305
1	2.763398	-2.162812	1.709078
77	0.243364	0.177828	-0.022799
6	-1.349162	-1.338430	0.775017
6	-2.420781	-2.147652	0.016690
1	-0.831263	-0.925824	-0.534231
1	-1.850640	-0.588878	1.397693
1	-1.920656	-2.905927	-0.601548
1	-2.996626	-2.696938	0.774489
6	-0.142978	-1.747118	2.782312
1	-0.957685	-1.381349	3.426726
1	0.558202	-0.925109	2.592891
6	-3.367372	-1.310921	-0.849111
1	-3.862667	-0.556193	-0.220531
1	-2.786208	-0.756818	-1.597856
6	-4.431245	-2.161925	-1.552139
1	-5.095486	-1.542729	-2.165800
1	-3.967743	-2.907075	-2.210120
1	-5.052922	-2.701893	-0.827460
1	0.367848	-2.569875	3.289380

Structure 11 - NBE

B3LYP/GBS(1) = -1429.659023 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.960543 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.725976 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.034754 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.077294 a.u.
Enthalpy Correction = 0.417602
Gibbs Free Energy Correction = 0.335762

Atomic No	x-coord	y-coord	z-coord
7	1.600105	-1.157770	-1.153722
6	2.812250	-0.581844	-1.441346
6	3.225653	0.583248	-0.871983
1	3.452386	-1.109660	-2.154946
1	4.189142	1.017907	-1.120943
6	1.261880	-2.400332	-1.635509
6	0.122029	-3.044320	-1.268372
1	1.964119	-2.864674	-2.334612
1	-0.122551	-4.021593	-1.674025
15	2.085374	1.310368	0.321562
15	-0.934000	-2.159045	-0.100520

8	-2.492158	0.588774	1.105620
6	1.895089	3.090501	-0.155525
1	1.241273	3.600651	0.560029
1	2.865416	3.599761	-0.173830
1	1.442785	3.155708	-1.148902
6	3.006240	1.450983	1.920533
1	3.943169	2.004591	1.792054
1	2.385018	1.963900	2.662145
1	3.227992	0.445926	2.288500
6	-2.620689	-2.110907	-0.855631
1	-3.029034	-3.120483	-0.978943
1	-3.274202	-1.514442	-0.213225
1	-2.561621	-1.629404	-1.835659
6	-1.196427	-3.280478	1.346722
1	-1.907611	-2.820572	2.040421
1	-1.586678	-4.253547	1.027530
1	-0.245211	-3.425247	1.865377
77	0.309713	-0.207335	0.232254
6	-1.306767	1.136355	0.526022
6	-1.703574	1.651863	-0.862869
1	0.025931	-0.138893	1.785985
1	-0.993245	1.987850	1.150777
1	-0.803951	2.000321	-1.386978
1	-2.106957	0.820318	-1.455849
6	-2.492492	0.532633	2.510178
1	-2.333183	1.527452	2.957084
1	-1.707724	-0.141938	2.889361
1	-3.473069	0.159082	2.821370
6	-2.739389	2.792284	-0.827149
6	-3.143498	3.275031	-2.223997
1	-2.328883	3.635133	-0.252147
1	-3.622592	2.444289	-0.279327
1	-3.881419	4.084470	-2.170520
1	-2.277420	3.651302	-2.783476
1	-3.585696	2.460842	-2.811829

Structure 11-12TS - NBE

B3LYP/GBS(1) = -1429.616730 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.924326 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.699594 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.005722 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.046214 a.u.
Enthalpy Correction = 0.412147
Gibbs Free Energy Correction = 0.33408
Imaginary Freq = -840.2 i

Atomic No	x-coord	y-coord	z-coord
7	0.903459	-2.160018	-0.509138
6	2.243554	-2.359212	-0.597179
6	3.151894	-1.369541	-0.373017
1	2.575586	-3.371493	-0.847759
1	4.218310	-1.545606	-0.476633

6	0.060924	-3.224010	-0.518911
6	-1.260796	-3.106520	-0.228515
1	0.495102	-4.199207	-0.759820
1	-1.926519	-3.963922	-0.268953
15	2.474320	0.225377	0.061623
15	-1.869064	-1.464216	0.157354
8	0.771845	2.575197	0.238862
6	3.239363	1.397667	-1.152980
1	3.086426	2.435935	-0.851353
1	4.315584	1.201861	-1.224443
1	2.785427	1.237703	-2.134637
6	3.253820	0.767207	1.647088
1	4.345458	0.812237	1.558727
1	2.869437	1.755034	1.917574
1	2.982458	0.056256	2.431247
6	-3.359516	-1.377341	-0.960136
1	-3.864973	-2.349510	-0.933640
1	-4.074524	-0.608381	-0.659853
1	-3.033955	-1.184840	-1.986451
6	-2.696918	-1.601162	1.812648
1	-3.192173	-0.661088	2.079215
1	-3.441253	-2.405935	1.814023
1	-1.931354	-1.813912	2.562679
77	0.163994	-0.184792	0.075202
6	-0.293844	1.722301	0.055919
6	-1.586431	2.520385	-0.056875
1	0.399667	-0.870070	1.529596
1	-0.136707	0.910584	-1.351583
1	-1.654860	3.091618	0.883148
6	0.764115	3.947597	-0.169067
1	0.039988	4.547979	0.391108
1	0.570791	4.045661	-1.244361
1	1.769315	4.315752	0.047185
6	-2.901871	1.795185	-0.289831
1	-2.832747	1.222467	-1.219166
1	-3.068587	1.079112	0.519854
6	-4.087226	2.765401	-0.366874
1	-4.196595	3.339108	0.561931
1	-3.964149	3.483260	-1.187472
1	-5.027179	2.227801	-0.536766
1	-1.475773	3.274002	-0.849168

Structure 11-13TS - NBE

B3LYP/GBS(1) = -1429.633819 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.943998 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.720183 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.027133 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.067116 a.u.
Enthalpy Correction = 0.412373
Gibbs Free Energy Correction = 0.33505
Imaginary Freq = -788.8i

Atomic No	x-coord	y-coord	z-coord
7	0.840652	2.018480	0.528684
6	2.170851	2.248484	0.652872

6	3.112511	1.292770	0.398534
1	2.471287	3.253302	0.964632
1	4.171854	1.500629	0.513786
6	-0.070378	3.015159	0.679817
6	-1.400287	2.831651	0.450831
1	0.312854	3.991527	0.990866
1	-2.109114	3.643582	0.585134
15	2.486673	-0.286737	-0.157957
15	-1.901442	1.201430	-0.108825
8	-1.729417	-2.082028	-1.208321
6	3.254496	-1.582016	0.925701
1	2.999547	-2.587737	0.572517
1	4.346013	-1.484045	0.928752
1	2.886785	-1.460210	1.948492
6	3.284568	-0.671818	-1.782188
1	4.377785	-0.663808	-1.701730
1	2.962423	-1.657834	-2.135478
1	2.967469	0.079159	-2.509593
6	-3.326682	0.727283	0.977717
1	-4.064687	1.537742	1.001081
1	-3.812268	-0.176708	0.597004
1	-2.972453	0.544006	1.995405
6	-2.790701	1.454704	-1.711728
1	-3.221070	0.508721	-2.053921
1	-3.596100	2.189389	-1.596340
1	-2.079155	1.813356	-2.459108
77	0.173367	0.074219	-0.114468
6	-0.447979	-1.889396	-0.664128
6	-0.357767	-1.971163	0.784942
1	0.343218	0.675272	-1.635690
1	0.308758	-2.444991	-1.226554
6	-1.737780	-1.959441	-2.615923
1	-1.097079	-2.721807	-3.088013
1	-1.386534	-0.966992	-2.930302
1	-0.019463	-0.550185	1.481078
1	0.557641	-2.438567	1.142647
6	-1.565996	-2.345206	1.624838
1	-2.449195	-1.815981	1.265539
1	-1.754523	-3.410652	1.421306
6	-1.382921	-2.135289	3.129215
1	-1.231114	-1.075357	3.365038
1	-2.261324	-2.484683	3.683515
1	-0.511622	-2.685569	3.506151
1	-2.768542	-2.114312	-2.947676

Structure 11-14TS - NBE

B3LYP/GBS(1) = -1429.613439 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.920538 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.699536 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1429.999019 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.039339 a.u.
Enthalpy Correction = 0.415782
Gibbs Free Energy Correction = 0.337915
Imaginary Freq = -179.4 i

Atomic No	x-coord	y-coord	z-coord
7	-1.553566	-1.591125	0.460298
6	-2.843359	-1.265228	0.765377
6	-3.349315	-0.012305	0.606545
1	-3.454232	-2.080050	1.156333
1	-4.378192	0.214558	0.866827
6	-1.103944	-2.875327	0.598673
6	0.161393	-3.254981	0.282185
1	-1.832069	-3.586736	0.990742
1	0.486054	-4.282233	0.415308
15	-2.196030	1.190590	-0.040998
15	1.231909	-1.942299	-0.303903
8	2.229282	0.941539	1.298328
6	-2.270631	2.664485	1.079243
1	-1.624676	3.465032	0.702258
1	-3.295314	3.046812	1.151346
1	-1.924439	2.376473	2.075227
6	-2.909666	1.893277	-1.599046
1	-3.904027	2.319670	-1.423261
1	-2.254775	2.678154	-1.993852
1	-2.982893	1.093438	-2.339861
6	2.802676	-2.083639	0.663812
1	3.283547	-3.049061	0.467565
1	3.481311	-1.270539	0.394712
1	2.578734	-2.004927	1.729360
6	1.833359	-2.401499	-1.995254
1	2.553846	-1.655048	-2.348690
1	2.320260	-3.383436	-1.988638
1	0.982570	-2.420501	-2.680102
77	-0.289577	-0.150883	-0.234167
6	1.008372	1.319744	0.655875
1	0.544618	2.106645	1.264401
6	2.022524	0.621487	2.650406
1	1.308144	-0.210849	2.762103
1	1.627582	1.482559	3.217079
6	1.302013	1.878468	-0.767875
1	0.665604	2.755214	-0.939026
1	0.994981	1.151990	-1.571287
1	-0.929180	-0.778600	-1.619885
6	2.770538	2.239918	-1.075186
1	3.408286	1.377747	-0.855181
1	2.860633	2.439405	-2.151813
6	3.262865	3.455624	-0.283329
1	3.234705	3.249520	0.789964
1	4.294827	3.707239	-0.556348
1	2.642478	4.338858	-0.483822
1	2.990617	0.337741	3.075641

Structure 11-15TS - NBE

B3LYP/GBS(1) = -1429.615542 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.925838 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.702180 a.u.

TPSS/GBS(2)//B3LYP/GBS(1) = -1430.006249 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.047040 a.u.
Enthalpy Correction = 0.41317
Gibbs Free Energy Correction = 0.335026
Imaginary Freq = -244.9 i

Atomic No	x-coord	y-coord	z-coord
7	-1.154383	-1.697613	-0.965093
6	-0.502795	-2.868777	-1.211760
6	0.721165	-3.152977	-0.694519
1	-1.024059	-3.581937	-1.853546
1	1.226621	-4.087089	-0.919123
6	-2.438283	-1.531973	-1.398178
6	-3.190725	-0.449034	-1.073630
1	-2.837201	-2.330384	-2.027152
1	-4.202605	-0.332083	-1.449010
15	1.437397	-1.882891	0.340640
15	-2.382728	0.766020	-0.036921
8	0.126606	2.666052	-0.023083
6	3.173074	-1.712934	-0.303925
1	3.813286	-1.158258	0.389155
1	3.604349	-2.710613	-0.446899
1	3.154677	-1.195220	-1.266304
6	1.772715	-2.627300	2.003661
1	2.401229	-3.521187	1.917660
1	2.278436	-1.898371	2.646747
1	0.818493	-2.894703	2.463104
6	-2.664991	2.384955	-0.886737
1	-3.716208	2.458620	-1.189930
1	-2.421462	3.217126	-0.222427
1	-2.023092	2.446220	-1.767691
6	-3.405245	0.981930	1.490512
1	-2.967304	1.762570	2.121959
1	-4.434912	1.262990	1.240963
1	-3.407017	0.041638	2.046582
77	-0.282600	-0.256304	0.255551
6	0.799918	1.455406	0.113680
6	2.309476	1.635141	0.209088
1	-1.026618	-1.213912	1.369147
1	0.439416	0.959463	1.333573
1	2.760929	0.699817	0.540589
1	2.593957	2.389446	0.959600
6	0.527252	3.793942	0.752844
1	1.484777	4.217138	0.425750
1	0.590872	3.541117	1.821202
6	2.908871	2.044112	-1.149467
1	2.418716	2.960740	-1.501520
1	2.662565	1.269483	-1.886407
6	4.425044	2.257028	-1.089865
1	4.689883	3.050692	-0.379803
1	4.943598	1.344028	-0.771159
1	4.825613	2.540867	-2.069942
1	-0.251811	4.548026	0.611737

Structure 12 - NBE

B3LYP/GBS(1) = -1429.653850 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.959875 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.729870 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.041233 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.080510 a.u.
Enthalpy Correction = 0.414196
Gibbs Free Energy Correction = 0.334219

Atomic No	x-coord	y-coord	z-coord
7	-1.682961	1.732958	-0.206066
6	-2.985723	1.448155	-0.454116
6	-3.448768	0.170242	-0.552476
1	-3.664646	2.297036	-0.577548
1	-4.496523	-0.039748	-0.744772
6	-1.246693	3.014483	-0.128326
6	0.061867	3.331670	0.086001
1	-1.997362	3.801539	-0.246204
1	0.393143	4.363551	0.148421
15	-2.240586	-1.126156	-0.303134
15	1.185549	1.948973	0.224275
8	1.239275	-2.264575	1.056873
6	-2.319254	-2.251211	-1.770043
1	-1.657095	-3.111861	-1.622748
1	-3.340335	-2.614467	-1.934710
1	-1.981722	-1.697040	-2.648637
6	-2.961938	-2.217993	1.010505
1	-3.996885	-2.476634	0.758130
1	-2.388020	-3.145085	1.109375
1	-2.948949	-1.684559	1.964130
6	2.513068	2.226941	-1.035982
1	2.956362	3.222276	-0.915017
1	3.305698	1.477317	-0.939765
1	2.069165	2.148231	-2.031346
6	2.130033	2.152822	1.801873
1	2.892994	1.371494	1.889580
1	2.619782	3.132644	1.845100
1	1.432187	2.056491	2.636829
77	-0.264225	0.108140	0.026219
6	1.079078	-1.298250	0.157788
6	2.200877	-1.492056	-0.859459
1	1.954256	-2.408190	-1.419684
1	2.161127	-0.674104	-1.578863
6	0.403888	-2.426103	2.212617
1	-0.096934	-1.486530	2.450480
1	1.067000	-2.752768	3.017271
6	3.615660	-1.637191	-0.265565
6	4.680081	-1.815418	-1.353506
1	3.639283	-2.487168	0.424037
1	3.851156	-0.746228	0.333958
1	5.681923	-1.904031	-0.917862
1	4.491973	-2.719487	-1.945535
1	4.690729	-0.964741	-2.046055
1	-0.328782	-3.210787	2.006360
1	-0.561121	0.201970	1.684865
1	-0.044045	0.131169	-1.644173

Structure 13 - NBE

B3LYP/GBS(1) = -1429.653990 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.963466 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.738885 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.046885 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.085326 a.u.
Enthalpy Correction = 0.414518
Gibbs Free Energy Correction = 0.336534

Atomic No	x-coord	y-coord	z-coord
7	1.204944	1.964437	-0.043004
6	2.563393	1.988839	-0.018859
6	3.326184	0.859601	-0.010789
1	3.030158	2.976945	-0.005228
1	4.410229	0.910401	0.005626
6	0.477919	3.116443	-0.028727
6	-0.880825	3.127131	-0.048494
1	1.047581	4.048637	-0.001130
1	-1.435499	4.060524	-0.046981
15	2.415947	-0.678163	-0.031910
15	-1.678536	1.521200	-0.127582
8	-1.890732	-1.682670	1.438236
6	3.015858	-1.693709	1.396343
1	2.546581	-2.684324	1.386770
1	4.103276	-1.825322	1.357788
1	2.746230	-1.184152	2.324774
6	3.033800	-1.671565	-1.466185
1	4.118081	-1.820599	-1.406892
1	2.546951	-2.653096	-1.489545
1	2.789341	-1.137781	-2.387632
6	-2.942351	1.485355	1.220909
1	-3.667830	2.298298	1.102761
1	-3.464953	0.524701	1.206891
1	-2.432696	1.593636	2.181394
6	-2.755372	1.596911	-1.632993
1	-3.407815	0.721305	-1.695422
1	-3.377063	2.499549	-1.610022
1	-2.114061	1.622934	-2.517413
77	0.207576	0.106228	-0.053843
6	-0.697355	-1.770980	0.757802
1	0.084732	-2.280199	1.318597
6	-1.754502	-1.482938	2.835719
1	-1.258031	-0.526783	3.043645
1	-1.172639	-2.295180	3.295936
6	-0.710292	-1.820984	-0.654965
1	0.089455	-2.403949	-1.106435
6	-2.003011	-1.874306	-1.443625
6	-2.484255	-3.323202	-1.635303
1	-1.859400	-1.400333	-2.420434
1	-2.780120	-1.310504	-0.920536
1	-3.411485	-3.354197	-2.220103
1	-1.736240	-3.924525	-2.166850
1	-2.677316	-3.802535	-0.669004
1	-2.763627	-1.485834	3.254350

1	0.297488	0.204582	-1.724345
1	0.260230	0.293397	1.617897

Structure 14 - NBE

B3LYP/GBS(1) = -1429.658987 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.966348 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.738310 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.047243 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.086822 a.u.
Enthalpy Correction = 0.415565
Gibbs Free Energy Correction = 0.336849

Atomic No	x-coord	y-coord	z-coord
7	-0.482504	-1.439129	1.243696
6	-1.715444	-1.525514	1.806554
6	-2.786025	-0.806150	1.354175
1	-1.830431	-2.213905	2.650499
1	-3.754548	-0.888883	1.839552
6	0.504117	-2.332276	1.524079
6	1.675171	-2.377884	0.824100
1	0.324244	-3.028639	2.349916
1	2.453631	-3.087172	1.092239
15	-2.521331	0.180168	-0.125338
15	1.834970	-1.253977	-0.578123
8	1.664508	1.434289	1.726959
6	-3.235860	1.856400	0.227750
1	-3.213101	2.474174	-0.676707
1	-4.274878	1.766851	0.564695
1	-2.659324	2.358992	1.009950
6	-3.701759	-0.427601	-1.412174
1	-4.736692	-0.393657	-1.052751
1	-3.612301	0.187634	-2.313769
1	-3.438553	-1.457027	-1.666815
6	3.495159	-0.450651	-0.392520
1	4.267465	-1.210614	-0.225168
1	3.744412	0.108232	-1.300659
1	3.472484	0.239632	0.452772
6	2.137552	-2.306015	-2.069726
1	2.288095	-1.664243	-2.944368
1	3.019119	-2.943397	-1.935268
1	1.258578	-2.930559	-2.244933
77	-0.237109	-0.157987	-0.500118
6	0.438074	1.526194	1.122336
1	-0.408426	1.466040	1.803882
6	1.700197	0.736340	2.967648
1	1.696805	-0.345105	2.806208
1	0.848978	1.018032	3.602510
6	0.325412	2.091182	-0.137565
1	-0.632825	2.543595	-0.369623
1	-0.165266	0.489490	-1.981872
1	-0.723870	-1.443788	-1.340917
6	1.500059	2.669440	-0.894484

1	2.389092	2.056452	-0.730368
1	1.284337	2.635333	-1.967884
6	1.793508	4.118667	-0.465680
1	2.056884	4.165054	0.596687
1	2.628508	4.535212	-1.041698
1	0.922917	4.766705	-0.626053
1	2.627969	1.034496	3.462406

Structure 15 - NBE

B3LYP/GBS(1) = -1429.654107 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.959578 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.731230 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.041351 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.080191 a.u.
Enthalpy Correction = 0.415128
Gibbs Free Energy Correction = 0.335752

Atomic No	x-coord	y-coord	z-coord
7	-0.138378	0.004534	-1.799286
6	1.003706	-0.185319	-2.509888
6	2.145414	-0.681774	-1.946643
1	0.978853	0.068802	-3.574935
1	3.049349	-0.804592	-2.536806
6	-1.327913	0.264586	-2.400911
6	-2.516979	0.221501	-1.727406
1	-1.306570	0.510436	-3.467989
1	-3.450401	0.460101	-2.229497
15	2.044623	-1.187406	-0.223156
15	-2.452891	-0.326724	-0.016649
8	0.578393	1.699618	2.183514
6	3.512297	-0.425434	0.618058
1	3.599477	-0.801597	1.643273
1	4.435462	-0.668942	0.079174
1	3.396773	0.661265	0.648277
6	2.495943	-2.977432	-0.141544
1	3.491270	-3.156491	-0.564703
1	2.480766	-3.312499	0.900935
1	1.749869	-3.546962	-0.699476
6	-3.430879	0.894013	0.977978
1	-4.448511	0.995955	0.583110
1	-3.488032	0.560581	2.019602
1	-2.940446	1.870614	0.949092
6	-3.519053	-1.827467	0.134974
1	-3.525373	-2.168626	1.175498
1	-4.546864	-1.616139	-0.182411
1	-3.095562	-2.618017	-0.487859
77	-0.157590	-0.576946	0.303291
6	0.164587	1.289257	0.991948
6	-0.050027	2.547073	0.168657
1	-0.477667	-2.140318	-0.203883
1	-0.215859	-1.192168	1.792298
1	-0.749952	2.331666	-0.642331

1	-0.477946	3.333567	0.807115
6	0.902712	0.767464	3.228633
1	1.639180	0.043191	2.880023
1	0.003482	0.236839	3.545251
6	1.278486	3.062892	-0.430789
1	1.977884	3.279578	0.387011
1	1.727604	2.269503	-1.038936
6	1.077188	4.318536	-1.284972
1	2.028985	4.667206	-1.702410
1	0.397430	4.121356	-2.122726
1	0.649826	5.138754	-0.695169
1	1.304019	1.377651	4.040488

Structure 15-16TS – NBE (Despite every attempt, full Convergence could not be obtained for this structure)

B3LYP/GBS(1) = -1429.597894 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.905877 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.666876 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1429.989267 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.033321 a.u.
Enthalpy Correction = 0.410423
Gibbs Free Energy Correction = 0.332256
Imaginary Freq = -866.5 i

Atomic No	x-coord	y-coord	z-coord
7	-0.338133	-1.784203	1.152021
6	0.736310	-2.436941	1.662164
6	2.010947	-2.137253	1.288881
1	0.539411	-3.228402	2.392009
1	2.865512	-2.650292	1.719472
6	-1.602884	-2.172231	1.454972
6	-2.701341	-1.610873	0.877359
1	-1.710869	-2.975524	2.190466
1	-3.704214	-1.929387	1.146956
15	2.197212	-0.806260	0.101208
15	-2.406231	-0.314263	-0.324567
6	3.282150	-1.484960	-1.240766
1	3.608762	-0.700685	-1.930586
1	4.169677	-1.967606	-0.815877
1	2.704864	-2.224406	-1.803901
6	3.323674	0.398975	0.957558
1	4.289802	-0.069449	1.178542
1	3.487071	1.302610	0.363306
1	2.842144	0.686287	1.896239
6	-3.204025	-0.835558	-1.915179
1	-4.259629	-1.089590	-1.766772
1	-3.131578	-0.025047	-2.648916
1	-2.672558	-1.707273	-2.304265
6	-3.594272	1.031087	0.167435
1	-3.646930	1.811026	-0.599083
1	-4.593295	0.594052	0.282698
1	-3.298261	1.477910	1.119033

77	-0.036176	-0.236158	-0.389936
6	0.197518	1.717464	-0.424957
6	-0.770052	2.666599	1.781324
6	0.525601	3.055395	2.502058
1	-1.060899	1.645018	2.048261
1	-1.576595	3.331949	2.120902
1	0.395935	3.009250	3.589748
1	1.356142	2.390090	2.239775
1	0.827129	4.078655	2.244677
1	0.076612	-0.776518	-2.006036
1	-0.110434	-1.666131	-1.500568
6	1.991778	1.871559	-2.060349
1	2.880983	1.415108	-1.620050
1	1.441803	1.118214	-2.631643
1	2.298922	2.704674	-2.698334
8	1.154870	2.439358	-1.058771
6	-0.686564	2.767129	0.246068
1	-0.330009	3.766498	-0.035761
1	-1.693712	2.663211	-0.168241

Structure 16 - NBE

B3LYP/GBS(1) = -1428.462214 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1428.758866 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1427.516349 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1428.834919 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1428.87803 a.u.
Enthalpy Correction = 0.39738
Gibbs Free Energy Correction = 0.315576

Atomic No	x-coord	y-coord	z-coord
7	-1.898117	1.408760	-0.452167
6	-3.134338	0.885633	-0.671639
6	-3.383456	-0.453839	-0.598811
1	-3.937774	1.588743	-0.912049
1	-4.375223	-0.858148	-0.776693
6	-1.695720	2.752634	-0.512935
6	-0.475816	3.317814	-0.281896
1	-2.561461	3.376663	-0.755439
1	-0.327797	4.392027	-0.335705
15	-1.967826	-1.468284	-0.187908
15	0.839732	2.163336	0.092235
8	1.639954	-1.633511	1.519891
6	-1.825858	-2.764091	-1.507201
1	-1.024374	-3.469455	-1.261151
1	-2.764747	-3.319628	-1.616456
1	-1.585072	-2.278717	-2.456549
6	-2.462488	-2.509607	1.266724
1	-3.386113	-3.061344	1.055158
1	-1.672009	-3.228368	1.509779
1	-2.626363	-1.859832	2.130427
6	2.197502	2.498848	-1.126629
1	2.477495	3.558849	-1.116662

1	3.081640	1.897632	-0.889220
1	1.849413	2.231075	-2.127670
6	1.634460	2.736656	1.667502
1	2.503943	2.112404	1.900552
1	1.959653	3.780717	1.587993
1	0.910967	2.649761	2.482534
77	-0.247200	0.094491	0.033957
6	1.220491	-1.098820	0.363452
6	2.120182	-1.649063	-0.736161
1	1.928203	-2.731343	-0.814018
1	1.810478	-1.197266	-1.683054
6	0.963292	-1.285432	2.738411
1	0.270058	-0.460244	2.545271
1	1.730064	-1.009706	3.467910
6	3.628930	-1.431481	-0.505286
6	4.479274	-1.971797	-1.659306
1	3.922563	-1.911129	0.434659
1	3.822567	-0.357256	-0.380340
1	5.547170	-1.802184	-1.478910
1	4.330493	-3.050896	-1.789501
1	4.219358	-1.485376	-2.607503
1	0.421169	-2.166501	3.095731

Structure 17 - NBE

B3LYP/GBS(1) = -271.737562 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -271.832478 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -271.636361 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -271.868815 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -271.819094 a.u.
M06/GBS2//B3LYP/GBS(1) = -271.620499 a.u.
MP2/GBS2//B3LYP/GBS(1) = -271.0534467 a.u.
Enthalpy Correction = 0.151160
Gibbs Free Energy Correction = 0.109646

Atomic No	x-coord	y-coord	z-coord
6	2.738901	-0.378035	0.002485
1	3.110090	-1.404296	-0.041731
1	3.160093	0.191643	-0.838855
1	3.067286	0.083964	0.944024
8	1.325285	-0.450904	-0.077678
6	0.686005	0.754961	-0.168221
6	-0.610901	0.910774	0.114279
6	-1.540244	-0.172024	0.591014
6	-2.670584	-0.473635	-0.409052
1	-0.966177	-1.083622	0.786574
1	-1.989619	0.129976	1.549079
1	-3.347550	-1.242930	-0.018673
1	-3.267614	0.423250	-0.615519
1	-2.263902	-0.828602	-1.362466
1	1.304856	1.582585	-0.518525
1	-1.028800	1.903014	-0.045515

Structure 18 - NBE

B3LYP/GBS(1) = -1428.464569 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1428.762960 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1427.535235 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1428.841248 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1428.88242122 a.u.
Enthalpy Correction = 0.397224
Gibbs Free Energy Correction = 0.318903

Atomic No	x-coord	y-coord	z-coord
7	0.022825	2.160987	-0.091029
6	1.201178	2.846605	0.054783
6	2.393272	2.222128	0.241463
1	1.139629	3.937544	0.016677
1	3.316010	2.784337	0.347009
6	-1.151451	2.847221	-0.276091
6	-2.352311	2.226267	-0.412817
1	-1.076999	3.937444	-0.311872
1	-3.267406	2.791536	-0.559418
15	2.317453	0.426120	0.235849
15	-2.285904	0.433086	-0.312893
8	-1.111735	-2.152900	1.708946
6	3.156104	-0.132412	1.793547
1	3.218438	-1.226097	1.824326
1	4.169267	0.278981	1.864238
1	2.571487	0.208628	2.652277
6	3.564566	-0.088090	-1.039718
1	4.530433	0.392356	-0.845130
1	3.703789	-1.173712	-1.034164
1	3.209828	0.213704	-2.028613
6	-3.514698	-0.063268	0.978879
1	-4.521257	0.280561	0.713997
1	-3.510819	-1.151171	1.087286
1	-3.225254	0.382143	1.934385
6	-3.096820	-0.210419	-1.850783
1	-3.172488	-1.302250	-1.810277
1	-4.103454	0.207000	-1.966371
1	-2.491100	0.066087	-2.717831
77	0.007968	0.073426	-0.026092
6	-0.024035	-1.873180	0.888311
1	0.931310	-2.095673	1.374065
6	-0.961293	-1.672717	3.035329
1	-0.877337	-0.578637	3.057391
1	-0.070116	-2.106449	3.515463
6	-0.160082	-2.043222	-0.510180
1	-1.170759	-2.280184	-0.846251
6	0.908566	-2.691699	-1.368808
6	0.865759	-2.254466	-2.837335
1	0.777702	-3.785743	-1.320038
1	1.900407	-2.487890	-0.947417
1	1.640478	-2.758283	-3.427773
1	-0.104981	-2.497634	-3.287566
1	1.006964	-1.171914	-2.923851
1	-1.848962	-1.986766	3.590372

Structure 20 - NBE

B3LYP/GBS(1) = -1429.636866 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.936894 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.693882 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.004858 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.046562 a.u.
Enthalpy Correction = 0.420855
Gibbs Free Energy Correction = 0.337945

Atomic No	x-coord	y-coord	z-coord
7	-1.813248	1.537953	-0.264346
6	-1.540265	2.879775	-0.184257
6	-0.300245	3.366959	0.086537
1	-2.388067	3.546326	-0.354761
1	-0.113001	4.434629	0.142443
6	-3.077608	1.120321	-0.587805
6	-3.408283	-0.192193	-0.719217
1	-3.815057	1.910865	-0.739776
1	-4.417927	-0.498437	-0.974313
15	0.946514	2.098636	0.301518
15	-2.047267	-1.320071	-0.430802
6	1.796705	2.451091	1.913841
1	2.635059	1.759839	2.057538
1	2.182777	3.476805	1.943924
1	1.083906	2.311044	2.730870
6	2.308431	2.447518	-0.905396
1	2.757456	3.432712	-0.731589
1	3.073790	1.670497	-0.820488
1	1.893954	2.412261	-1.916454
6	-2.663575	-2.554090	0.813486
1	-3.594407	-3.023334	0.473546
1	-1.915378	-3.337436	0.977845
1	-2.847312	-2.043081	1.762327
6	-1.918576	-2.396920	-1.938543
1	-1.157958	-3.171379	-1.787298
1	-2.875078	-2.883183	-2.164011
1	-1.620055	-1.778327	-2.788969
77	-0.339156	0.186343	0.036543
6	1.800058	-1.526417	0.626792
6	1.316282	-2.643411	1.560822
1	0.967368	-1.203748	-0.082970
1	2.175824	-0.678753	1.202505
1	0.676966	-3.336951	0.998396
1	2.187667	-3.230087	1.886827
6	0.571908	-2.117419	2.791934
1	1.248957	-1.547538	3.440092
1	-0.239183	-1.443532	2.490033
6	4.315306	-1.243171	-2.059103
1	4.581618	-0.333197	-2.602387
1	5.220454	-1.654912	-1.583370
1	3.930513	-1.987073	-2.774647

1	0.153183	-2.939065	3.384292
6	2.895256	-1.985811	-0.335466
8	3.338554	-0.887270	-1.103746
1	3.733868	-2.408047	0.247073
1	2.518295	-2.788651	-0.992571

Structure 20-21TS - NBE

B3LYP/GBS(1) = -1429.625259 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.929427 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.688599 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.002629 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.046157 a.u.
Enthalpy Correction = 0.416397
Gibbs Free Energy Correction = 0.335355
Imaginary Freq = -641.8 i

Atomic No	x-coord	y-coord	z-coord
7	0.239778	-2.177822	0.458126
6	1.484839	-2.754372	0.435135
6	2.595749	-2.089234	0.022286
1	1.540432	-3.794799	0.764824
1	3.571390	-2.565397	0.020870
6	-0.856588	-2.929018	0.791261
6	-2.125262	-2.442376	0.734688
1	-0.661419	-3.958217	1.102734
1	-2.979281	-3.055792	1.004790
15	2.299574	-0.393580	-0.492715
15	-2.246431	-0.741576	0.172311
6	2.938193	-0.240058	-2.226559
1	2.850757	0.797643	-2.566937
1	3.989079	-0.545171	-2.290674
1	2.336946	-0.873767	-2.883474
6	3.517053	0.647688	0.435862
1	4.544016	0.319220	0.237276
1	3.410036	1.698857	0.152800
1	3.304654	0.563886	1.503565
6	-3.378033	-0.753118	-1.297763
1	-4.333227	-1.235203	-1.058950
1	-3.573614	0.270450	-1.635476
1	-2.892055	-1.300734	-2.109372
6	-3.313663	0.122382	1.423950
1	-3.523360	1.149332	1.104294
1	-4.265962	-0.403734	1.559087
1	-2.787276	0.155052	2.382139
77	0.003016	-0.221893	-0.147206
6	-0.143909	2.122650	-0.405292
6	-1.296207	2.832851	-1.152290
1	-0.241288	0.989647	-1.212596
1	0.807134	2.501901	-0.796619
1	-2.256846	2.463148	-0.766889
1	-1.259276	3.903882	-0.904277
6	-1.261457	2.675556	-2.675696

1	-0.322297	3.063490	-3.089404
1	-1.344960	1.623307	-2.971933
6	0.986989	2.506751	3.102123
1	0.240234	1.883932	3.620694
1	1.976877	2.283070	3.509305
1	0.752415	3.566477	3.300116
1	-2.084693	3.225234	-3.146208
6	-0.199753	2.504455	1.077838
1	-1.031468	1.998908	1.590048
1	-0.392749	3.595712	1.145867
8	1.028786	2.226571	1.721899

Structure 21 - NBE

B3LYP/GBS(1) = -1429.661237 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.963767 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.743394 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.040570 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.078511 a.u.
Enthalpy Correction = 0.417938
Gibbs Free Energy Correction = 0.339367

Atomic No	x-coord	y-coord	z-coord
7	0.386597	-2.155194	-0.118049
6	-0.690287	-2.983304	-0.128776
6	-1.972789	-2.515094	-0.167742
1	-0.493611	-4.060221	-0.108965
1	-2.816898	-3.198691	-0.180309
6	1.660302	-2.626329	-0.151468
6	2.748498	-1.801225	-0.215118
1	1.791089	-3.713171	-0.128830
1	3.756210	-2.205611	-0.238750
15	-2.169645	-0.730447	-0.241532
15	2.396777	-0.043169	-0.287198
6	-3.464508	-0.322619	1.027909
1	-3.702321	0.746159	1.001746
1	-4.382620	-0.891334	0.838459
1	-3.097080	-0.578419	2.025629
6	-3.104235	-0.365536	-1.799419
1	-4.042209	-0.931603	-1.837235
1	-3.330012	0.703834	-1.866730
1	-2.482641	-0.645261	-2.653702
6	3.391649	0.780454	1.038709
1	4.453288	0.520328	0.960867
1	3.285602	1.867992	0.961052
1	3.009723	0.465066	2.012462
6	3.190778	0.625482	-1.818379
1	3.038802	1.708769	-1.873537
1	4.266148	0.414235	-1.833822
1	2.720770	0.162459	-2.689852
77	0.069415	-0.013688	-0.136970
6	-0.151496	2.086091	0.173605
6	-1.197051	2.906901	-0.589148

1	0.039058	-0.070052	-1.704970
1	0.814915	2.594530	0.035797
1	-2.190437	2.448481	-0.469998
1	-1.282027	3.918426	-0.151244
6	-0.882429	3.055144	-2.080352
1	-0.819807	2.072771	-2.560413
1	0.083512	3.555469	-2.227369
6	-0.254461	0.357253	3.408582
1	0.266126	-0.578618	3.623256
1	0.008655	1.103647	4.172068
1	-1.340107	0.186360	3.440519
6	-0.454750	2.026738	1.669482
8	0.165198	0.793319	2.127773
1	-1.645270	3.650036	-2.597913
1	-0.065554	2.859446	2.279830
1	-1.538310	1.949225	1.846435

Structure 23 - NBE

B3LYP/GBS(1) = -1429.646875 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.957879 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.732042 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.041096 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.079303 a.u.
Enthalpy Correction = 0.414667
Gibbs Free Energy Correction = 0.335544

Atomic No	x-coord	y-coord	z-coord
7	-1.771213	1.473982	-0.523938
6	-3.014217	1.005685	-0.820326
6	-3.344670	-0.310721	-0.743497
1	-3.750311	1.751454	-1.129453
1	-4.344901	-0.656879	-0.984348
6	-1.493121	2.804218	-0.591739
6	-0.268184	3.317583	-0.301938
1	-2.316283	3.455481	-0.894758
1	-0.071665	4.382994	-0.369996
15	-2.039569	-1.407656	-0.198335
15	0.988730	2.124265	0.142820
6	-1.861635	-2.720197	-1.490637
1	-1.133992	-3.476054	-1.175414
1	-2.820842	-3.215205	-1.680492
1	-1.504135	-2.252322	-2.410773
6	-2.762722	-2.378894	1.203755
1	-3.732806	-2.797761	0.911732
1	-2.101742	-3.201914	1.492827
1	-2.900162	-1.716399	2.061822
6	2.399465	2.460783	-1.012421
1	2.628907	3.532709	-1.021342
1	3.299068	1.915259	-0.710482
1	2.114944	2.145565	-2.019423
6	1.713159	2.672747	1.755871
1	2.559434	2.035352	2.034928

1	2.063067	3.709516	1.694577
1	0.943841	2.592576	2.527489
77	-0.269006	0.124444	0.083196
6	1.267101	-1.453630	0.069852
1	0.801085	-2.415055	-0.142150
6	1.153449	-0.972673	1.395800
1	1.915093	-0.260438	1.711491
6	0.624640	-1.811069	2.536125
1	1.454858	-2.381212	2.979281
1	-0.124180	-2.532620	2.199755
1	0.175703	-1.196497	3.321268
6	2.492988	-1.222164	-0.773792
8	3.441442	-2.233893	-0.440535
6	4.600655	-2.171180	-1.238083
1	5.257263	-2.987858	-0.924615
1	4.369203	-2.291118	-2.309851
1	5.138076	-1.215872	-1.110554
1	2.248679	-1.274689	-1.845539
1	2.922020	-0.228348	-0.578788
1	-0.820195	0.502212	1.618952
1	0.031516	-0.023853	-1.561515

Structure 25 - NBE

B3LYP/GBS(1) = -1429.617834 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.925094 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.694202 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.005903 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.045736 a.u.
Enthalpy Correction = 0.413901
Gibbs Free Energy Correction = 0.334156

Atomic No	x-coord	y-coord	z-coord
7	-1.095490	0.882841	1.436743
6	-0.644840	2.071884	1.913798
6	0.279851	2.830160	1.250730
1	-1.061570	2.419487	2.865070
1	0.629730	3.770996	1.665867
6	-2.175805	0.253764	1.965791
6	-2.776448	-0.810867	1.353682
1	-2.565515	0.637001	2.914725
1	-3.624415	-1.312262	1.811677
15	0.801023	2.234611	-0.362521
15	-2.141158	-1.277496	-0.261310
6	2.652269	2.287624	-0.389029
1	3.020927	1.999582	-1.379326
1	3.013966	3.296729	-0.159819
1	3.049336	1.590548	0.353261
6	0.394670	3.534976	-1.608979
1	0.877508	4.487047	-1.359408
1	0.728550	3.208607	-2.599393
1	-0.689137	3.665241	-1.633377
6	-1.868292	-3.110192	-0.224919

1	-2.790403	-3.637636	0.045963
1	-1.540386	-3.457292	-1.210570
1	-1.094011	-3.349886	0.508777
6	-3.524545	-1.155481	-1.478106
1	-3.171330	-1.470027	-2.465738
1	-4.369193	-1.786614	-1.177983
1	-3.844824	-0.113394	-1.538028
77	-0.332760	0.185556	-0.479946
6	1.052780	-1.014137	0.276301
6	1.102097	-1.483834	1.702656
1	-1.500654	1.139986	-1.235469
1	0.155728	-0.214124	-1.970064
1	0.114300	-1.392412	2.161005
1	1.435277	-2.528805	1.753490
6	2.107833	-0.625472	2.513760
1	3.119400	-0.727757	2.111832
1	1.815949	0.428799	2.500879
6	4.104255	-2.867209	-0.769420
1	4.644382	-2.088074	-1.331957
1	4.818692	-3.417014	-0.150893
1	3.650593	-3.561479	-1.495659
8	3.138467	-2.313942	0.096967
6	2.145828	-1.572220	-0.596242
1	1.641123	-2.211679	-1.343557
1	2.605641	-0.755945	-1.176015
1	2.117691	-0.966529	3.554916

Structure 26 - NBE

B3LYP/GBS(1) = -1428.426981 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1428.724615 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1427.484906 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1428.799058 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1428.842736 a.u.
Enthalpy Correction = 0.396463
Gibbs Free Energy Correction = 0.315017

Atomic No	x-coord	y-coord	z-coord
7	0.848720	2.107516	-0.371010
6	-0.011248	3.161107	-0.277576
6	-1.318497	3.005112	0.068651
1	0.396029	4.155350	-0.485625
1	-1.993519	3.852933	0.134669
6	2.155576	2.313271	-0.693244
6	3.058641	1.294555	-0.766610
1	2.461526	3.343341	-0.900958
1	4.097722	1.472624	-1.025749
15	-1.845974	1.313606	0.341970
15	2.414572	-0.324557	-0.357068
6	-3.291740	1.058691	-0.785314
1	-3.745673	0.081637	-0.605277
1	-4.035780	1.847817	-0.624374
1	-2.944305	1.089975	-1.820305

6	-2.677773	1.273750	1.999426
1	-3.480028	2.018840	2.055088
1	-3.103711	0.281272	2.182444
1	-1.937718	1.484824	2.775678
6	2.903823	-1.470290	-1.730247
1	3.984877	-1.437409	-1.909492
1	2.616532	-2.498684	-1.484779
1	2.378452	-1.171007	-2.640917
6	3.475836	-0.956884	1.028076
1	3.214479	-1.988053	1.286195
1	4.533295	-0.926284	0.740281
1	3.327920	-0.325495	1.907784
77	0.148011	0.095697	0.040319
6	-0.464357	-1.662457	0.399818
6	-1.535621	-2.413813	-0.347528
1	-1.093899	-3.376686	-0.678542
1	-2.335981	-2.695140	0.369905
6	0.145683	-1.916356	2.886594
1	-0.858136	-1.645353	3.232774
1	0.738944	-0.998554	2.849100
6	-3.001518	-2.524441	-2.168957
1	-3.366523	-1.918713	-3.002236
1	-2.529359	-3.436064	-2.570611
1	-3.859056	-2.829364	-1.545428
1	0.583110	-2.601683	3.622872
6	0.083260	-2.576326	1.500563
8	-2.080884	-1.732558	-1.450435
1	-0.497990	-3.509942	1.573437
1	1.096643	-2.882269	1.204615

Structure 27 - NBE

B3LYP/GBS(1) = -271.733252 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -271.829253 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -271.632096 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -271.864775 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -271.814884 a.u.
Enthalpy Correction = 0.150753
Gibbs Free Energy Correction = 0.110192

Atomic No	x-coord	y-coord	z-coord
6	2.942692	-0.010751	-0.178890
1	3.577083	-0.782482	-0.623375
1	3.061332	0.922471	-0.754427
1	3.280777	0.178659	0.853903
8	1.616692	-0.487105	-0.217526
6	0.693657	0.429474	0.352668
6	-0.671665	-0.189200	0.358625
6	-1.758579	0.378051	-0.169706
6	-3.141564	-0.206369	-0.142026
1	-3.535282	-0.338493	-1.158855
1	-3.156749	-1.180571	0.358001
1	-3.843696	0.456263	0.382336

1	0.687475	1.378612	-0.210773
1	-0.744494	-1.161086	0.847606
1	1.009290	0.669931	1.385671
1	-1.656521	1.346307	-0.663911

Structure 28 - NBE

B3LYP/GBS(1) = -1428.456022 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1428.755536 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1427.527069 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1428.832757 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1428.873653 a.u.
Enthalpy Correction = 0.397477
Gibbs Free Energy Correction = 0.315617

Atomic No	x-coord	y-coord	z-coord
7	0.410522	-1.930412	-0.943057
6	1.665666	-2.228714	-1.408913
6	2.743423	-1.438218	-1.171401
1	1.760753	-3.145301	-1.996806
1	3.728359	-1.692185	-1.550520
6	-0.636284	-2.765978	-1.236259
6	-1.905933	-2.526228	-0.818184
1	-0.399658	-3.652496	-1.830415
1	-2.720409	-3.201387	-1.061298
15	2.400614	0.020708	-0.182979
15	-2.110302	-1.013946	0.126676
6	3.012042	1.474444	-1.156805
1	2.963460	2.386112	-0.551835
1	4.047674	1.321327	-1.480560
1	2.370487	1.608939	-2.031348
6	3.640283	-0.032384	1.197604
1	4.652141	-0.164558	0.797189
1	3.613021	0.895582	1.777572
1	3.406432	-0.868692	1.861566
6	-3.465928	-0.082155	-0.732360
1	-4.328047	-0.734073	-0.915019
1	-3.792992	0.768132	-0.124928
1	-3.088038	0.293414	-1.686900
6	-2.959270	-1.502138	1.702406
1	-3.207611	-0.616833	2.297606
1	-3.882931	-2.053267	1.492457
1	-2.287871	-2.137518	2.286229
77	0.089443	-0.200888	0.182650
6	-0.071387	1.890959	0.717548
1	0.906767	2.370969	0.679048
6	-0.353233	1.100467	1.863803
1	-1.406437	1.009614	2.137310
6	0.564616	0.995161	3.059776
1	0.294231	1.740070	3.824657
1	1.608343	1.167895	2.783040
1	0.500380	0.005147	3.526506
6	-1.123415	2.709096	0.018838

8	-0.802153	2.851949	-1.356095
6	-1.679057	3.724757	-2.028216
1	-1.353754	3.774050	-3.071160
1	-2.721827	3.365698	-1.999229
1	-1.657512	4.741455	-1.599503
1	-2.118966	2.252639	0.137995
1	-1.173336	3.715113	0.482018

Structure 30 - NBE

B3LYP/GBS(1) = -1429.638269 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.939132 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.696462 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.007538 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.049246 a.u.
Enthalpy Correction = 0.420904
Gibbs Free Energy Correction = 0.337921

Atomic No	x-coord	y-coord	z-coord
7	1.625123	1.621270	-0.586738
6	2.877794	1.331377	-1.060302
6	3.394258	0.073008	-1.063219
1	3.450184	2.180100	-1.439737
1	4.390899	-0.128351	-1.442863
6	1.190361	2.921851	-0.571783
6	-0.028058	3.285072	-0.092996
1	1.888771	3.660683	-0.969454
1	-0.351678	4.321154	-0.098273
15	2.298897	-1.162677	-0.372693
15	-1.025743	1.914057	0.488751
6	3.248814	-2.024854	0.969110
1	2.663070	-2.856132	1.377286
1	4.199872	-2.418532	0.591357
1	3.449348	-1.311706	1.772971
6	2.162364	-2.522411	-1.630256
1	3.149704	-2.915443	-1.899957
1	1.554756	-3.345895	-1.236820
1	1.676387	-2.128275	-2.526774
6	-1.559481	2.327880	2.216991
1	-2.052050	3.306443	2.256969
1	-2.257835	1.568889	2.587150
1	-0.680640	2.340041	2.867018
6	-2.638477	2.050560	-0.421111
1	-3.324031	1.243463	-0.142296
1	-3.118272	3.014922	-0.215783
1	-2.437718	1.978153	-1.493892
77	0.451678	0.144884	0.145502
6	-1.028647	-2.016846	1.068813
6	-0.771092	-2.714910	2.409519
1	-0.616938	-0.964674	1.245480
1	-0.479428	-2.525804	0.273378
1	-1.298986	-2.208628	3.225978
1	-1.123344	-3.752831	2.374064

6	-2.513786	-1.903807	0.708532
1	-3.022474	-2.845151	0.956252
1	-2.988919	-1.125946	1.319718
6	-4.447238	-0.980012	-2.278750
1	-5.500242	-0.685928	-2.300196
1	-3.841965	-0.176945	-2.728643
1	-4.318231	-1.890389	-2.886830
1	0.295799	-2.721343	2.653353
6	-2.745475	-1.581285	-0.763623
8	-4.102683	-1.203104	-0.928712
1	-2.517328	-2.464215	-1.386949
1	-2.067641	-0.772248	-1.085744

Structure 30-31TS - NBE

B3LYP/GBS(1) = -1429.626802 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.931629 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.691637 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.005139 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.049164 a.u.
Enthalpy Correction = 0.416714
Gibbs Free Energy Correction = 0.337209
Imaginary Freq = -743.7 i

Atomic No	x-coord	y-coord	z-coord
7	1.337547	1.708376	-0.796204
6	2.603207	1.565166	-1.302131
6	3.312504	0.409508	-1.201049
1	3.029808	2.443165	-1.793877
1	4.314262	0.321601	-1.609672
6	0.745626	2.946937	-0.788004
6	-0.453227	3.179460	-0.196112
1	1.298679	3.751632	-1.278902
1	-0.912972	4.162842	-0.215522
15	2.480634	-0.893388	-0.291368
15	-1.232507	1.731243	0.531545
6	3.597975	-1.324168	1.124610
1	3.202141	-2.179303	1.682017
1	4.604005	-1.571108	0.765915
1	3.657784	-0.466344	1.799417
6	2.601557	-2.426783	-1.327977
1	3.644595	-2.659242	-1.571496
1	2.167556	-3.279038	-0.793296
1	2.044060	-2.276376	-2.256749
6	-1.593347	2.139611	2.303156
1	-2.167837	3.069355	2.385121
1	-2.166295	1.328272	2.765069
1	-0.648540	2.249112	2.841616
6	-2.941409	1.743981	-0.193712
1	-3.537126	0.891788	0.145727
1	-3.453599	2.674693	0.077701
1	-2.858931	1.696856	-1.283474
77	0.415846	0.107249	0.148327

6	-0.601669	-1.903831	0.663746
6	-0.098959	-2.852420	1.770555
1	-0.038038	-0.751561	1.439963
1	-0.253292	-2.308125	-0.293051
1	-0.431406	-2.529899	2.765525
1	-0.486318	-3.866907	1.605767
6	-2.134530	-1.835252	0.659025
1	-2.488943	-1.026328	1.309031
1	-2.552545	-2.763855	1.075649
6	-4.754107	-1.332615	-1.875468
1	-5.819052	-1.172733	-1.684878
1	-4.365417	-0.485648	-2.464174
1	-4.632365	-2.250608	-2.473534
1	0.993967	-2.906566	1.793893
6	-2.714540	-1.647490	-0.737439
1	-2.232715	-0.795809	-1.242741
1	-2.516705	-2.544881	-1.350335
8	-4.114262	-1.439028	-0.623291

Structure 31 - NBE

B3LYP/GBS(1) = -1429.648621 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.952095 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.727021 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.024836 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.066604 a.u.
Enthalpy Correction = 0.416912
Gibbs Free Energy Correction = 0.335501

Atomic No	x-coord	y-coord	z-coord
7	1.759555	1.574598	-0.620499
6	3.002059	1.192411	-1.018305
6	3.435539	-0.101819	-0.938757
1	3.660696	1.970307	-1.418117
1	4.435528	-0.377320	-1.260192
6	1.311070	2.850557	-0.779100
6	0.037295	3.222218	-0.461403
1	2.017981	3.583127	-1.181817
1	-0.295351	4.247577	-0.594469
15	2.258848	-1.288760	-0.287055
15	-1.045843	1.927998	0.161087
6	3.106046	-2.194744	1.090588
1	2.447300	-2.972897	1.490932
1	4.033924	-2.661477	0.740207
1	3.348227	-1.492443	1.893585
6	2.055751	-2.635589	-1.538835
1	3.019576	-3.094201	-1.786810
1	1.382307	-3.407069	-1.150061
1	1.616941	-2.212807	-2.446293
6	-1.749879	2.570785	1.751967
1	-2.222201	3.548015	1.598662
1	-2.497144	1.874696	2.146174
1	-0.947730	2.680403	2.487694

6	-2.540573	1.917256	-0.931320
1	-3.258555	1.157927	-0.604498
1	-3.025746	2.900146	-0.927872
1	-2.224502	1.684394	-1.951992
77	0.405170	0.070727	0.160102
6	-0.768794	-1.393087	1.146480
6	-0.426056	-1.211117	2.640019
1	-0.146226	-0.305237	-1.240763
1	-0.430294	-2.402726	0.861196
1	-0.784613	-0.245735	3.024323
1	-0.886036	-1.991492	3.268012
6	-2.292722	-1.368278	0.958901
1	-2.779418	-2.075214	1.651921
1	-2.690773	-0.377465	1.217268
8	-4.149098	-1.429561	-0.552935
6	-2.757499	-1.709333	-0.450664
6	-4.686035	-1.784006	-1.805782
1	-5.749729	-1.528708	-1.790612
1	-4.200630	-1.237222	-2.631785
1	-4.582364	-2.863818	-2.004772
1	0.656918	-1.256974	2.825332
1	-2.570855	-2.775262	-0.672089
1	-2.201744	-1.120274	-1.197260

Structure 33 - NBE

B3LYP/GBS(1) = -1429.646875 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.957879 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.732042 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.041096 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.079303 a.u.
Enthalpy Correction = 0.414667
Gibbs Free Energy Correction = 0.335544

Atomic No	x-coord	y-coord	z-coord
7	-1.771213	1.473982	-0.523938
6	-3.014217	1.005685	-0.820326
6	-3.344670	-0.310721	-0.743497
1	-3.750311	1.751454	-1.129453
1	-4.344901	-0.656879	-0.984348
6	-1.493121	2.804218	-0.591739
6	-0.268184	3.317583	-0.301938
1	-2.316283	3.455481	-0.894758
1	-0.071665	4.382994	-0.369996
15	-2.039569	-1.407656	-0.198335
15	0.988730	2.124265	0.142820
6	-1.861635	-2.720197	-1.490637
1	-1.133992	-3.476054	-1.175414
1	-2.820842	-3.215205	-1.680492
1	-1.504135	-2.252322	-2.410773
6	-2.762722	-2.378894	1.203755
1	-3.732806	-2.797761	0.911732
1	-2.101742	-3.201914	1.492827

1	-2.900162	-1.716399	2.061822
6	2.399465	2.460783	-1.012421
1	2.628907	3.532709	-1.021342
1	3.299068	1.915259	-0.710482
1	2.114944	2.145565	-2.019423
6	1.713159	2.672747	1.755871
1	2.559434	2.035352	2.034928
1	2.063067	3.709516	1.694577
1	0.943841	2.592576	2.527489
77	-0.269006	0.124444	0.083196
6	1.267101	-1.453630	0.069852
1	0.801085	-2.415055	-0.142150
6	1.153449	-0.972673	1.395800
1	1.915093	-0.260438	1.711491
6	0.624640	-1.811069	2.536125
1	1.454858	-2.381212	2.979281
1	-0.124180	-2.532620	2.199755
1	0.175703	-1.196497	3.321268
6	2.492988	-1.222164	-0.773792
8	3.441442	-2.233893	-0.440535
6	4.600655	-2.171180	-1.238083
1	5.257263	-2.987858	-0.924615
1	4.369203	-2.291118	-2.309851
1	5.138076	-1.215872	-1.110554
1	2.248679	-1.274689	-1.845539
1	2.922020	-0.228348	-0.578788
1	-0.820195	0.502212	1.618952
1	0.031516	-0.023853	-1.561515

Structure 36 - NBE

B3LYP/GBS(1) = -1428.431271 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1428.728715 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1427.494199 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1428.803846 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1428.847057 a.u.
Enthalpy Correction = 0.397006
Gibbs Free Energy Correction = 0.316281
Imaginary Freq = i

Atomic No	x-coord	y-coord	z-coord
7	-1.516757	1.670731	-0.699396
6	-2.769438	1.409038	-1.178787
6	-3.333203	0.172599	-1.110483
1	-3.310482	2.243049	-1.636194
1	-4.331721	-0.016752	-1.492644
6	-0.993097	2.931198	-0.785391
6	0.252470	3.234477	-0.331341
1	-1.626363	3.702438	-1.234416
1	0.656486	4.238913	-0.412646
15	-2.349286	-1.082628	-0.285115
15	1.194151	1.849712	0.319688
6	-2.309103	-2.553843	-1.413413

1	-1.806416	-3.392442	-0.919494
1	-3.321282	-2.864809	-1.697327
1	-1.747788	-2.293948	-2.314897
6	-3.448682	-1.706659	1.075081
1	-4.440008	-1.948033	0.674748
1	-3.033267	-2.605058	1.541777
1	-3.551582	-0.927850	1.835449
6	2.731352	1.799758	-0.720923
1	3.253499	2.762157	-0.664798
1	3.413282	1.004721	-0.405100
1	2.439302	1.618355	-1.758966
6	1.870683	2.396743	1.956001
1	2.538551	1.632025	2.367129
1	2.429033	3.334856	1.857117
1	1.040277	2.544539	2.651672
77	-0.366405	0.095222	0.200917
6	0.641033	-1.281186	1.050958
6	2.153876	-1.451074	0.922238
1	2.653910	-0.531416	1.249098
1	2.541619	-2.257545	1.561004
6	0.079475	-2.351773	1.958425
1	0.268677	-3.351021	1.529815
1	0.612242	-2.341015	2.922452
6	4.526232	-1.910837	-1.852637
1	5.611534	-1.786995	-1.800250
1	4.299583	-2.947038	-2.152902
1	4.126154	-1.234129	-2.625221
8	4.008101	-1.612956	-0.574830
6	2.593238	-1.724894	-0.518776
1	-0.987002	-2.247798	2.156847
1	2.116062	-1.009563	-1.203829
1	2.279347	-2.736720	-0.828874

Structure 37 - NBE

B3LYP/GBS(1) = -271.729724 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -271.826020 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -271.629755 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -271.861268 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -271.810969 a.u.
Enthalpy Correction = 0.151032
Gibbs Free Energy Correction = 0.110526

Atomic No	x-coord	y-coord	z-coord
6	-2.862532	-0.263831	0.172498
1	-3.694288	0.445422	0.197309
1	-3.023819	-0.973887	-0.655446
1	-2.850939	-0.833512	1.116239
8	-1.680286	0.485095	-0.002593
6	-0.520929	-0.324637	-0.052026
6	0.694764	0.586380	-0.232828
6	1.972786	-0.189932	-0.395763
6	3.014932	-0.135858	0.434341

1	3.913871	-0.722612	0.264679
1	-0.590138	-1.043628	-0.888152
1	0.513193	1.208684	-1.120542
1	-0.419207	-0.914888	0.874662
1	2.024240	-0.847468	-1.265781
1	0.763630	1.263866	0.626089
1	3.011615	0.504522	1.314364

Structure 38 - NBE

B3LYP/GBS(1) = -1428.456897 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1428.757208 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1427.529189 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1428.834096 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1428.87472503 a.u.
Enthalpy Correction = 0.397361
Gibbs Free Energy Correction = 0.317209

Atomic No	x-coord	y-coord	z-coord
7	1.272675	1.237804	1.297177
6	2.442498	0.795211	1.861966
6	3.075942	-0.336095	1.452869
1	2.852614	1.404173	2.671890
1	3.996681	-0.670407	1.920454
6	0.717607	2.423965	1.711128
6	-0.399523	2.946995	1.144109
1	1.227795	2.941285	2.527846
1	-0.824171	3.883529	1.492600
15	2.266847	-1.190435	0.097539
15	-1.103354	1.971709	-0.193850
6	2.074870	-2.956464	0.629836
1	1.665878	-3.559599	-0.188118
1	3.038528	-3.382299	0.931197
1	1.383148	-3.000614	1.475467
6	3.516972	-1.353717	-1.261478
1	4.417508	-1.872374	-0.913208
1	3.088810	-1.914871	-2.099640
1	3.790403	-0.355694	-1.614178
6	-2.908245	1.838841	0.215577
1	-3.317499	2.827982	0.451564
1	-3.467359	1.419790	-0.626599
1	-3.042717	1.182372	1.078939
6	-1.159394	3.085503	-1.675761
1	-1.664481	2.582910	-2.507764
1	-1.691897	4.016589	-1.451615
1	-0.136110	3.320069	-1.980669
77	0.402166	0.161889	-0.257676
6	-0.685105	-1.395125	-1.335720
1	-0.161722	-2.343547	-1.203162
6	-0.118044	-0.475339	-2.252530
1	-0.765983	0.229425	-2.772405
6	-2.172164	-1.516101	-1.083226
1	-2.675747	-0.567311	-1.296142

1	-2.602490	-2.259759	-1.772502
6	-2.500439	-1.944781	0.342863
1	-2.043481	-2.927483	0.559543
1	-2.075051	-1.225033	1.061222
8	-3.909936	-2.021308	0.482158
6	-4.306771	-2.444162	1.765458
1	-5.400333	-2.467335	1.778631
1	-3.926808	-3.452674	2.000628
1	-3.955564	-1.756182	2.552863
1	0.772433	-0.744088	-2.819159

Structure 40 - NBE

B3LYP/GBS(1) = -1429.640730 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.944726 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.700554 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.013018 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.055496 a.u.
Enthalpy Correction = 0.420594
Gibbs Free Energy Correction = 0.33609

Atomic No	x-coord	y-coord	z-coord
7	2.712497	0.772009	-0.279075
6	3.791551	-0.064007	-0.397280
6	3.690746	-1.416958	-0.296902
1	4.752875	0.421069	-0.578027
1	4.561117	-2.058041	-0.394281
6	2.891004	2.126955	-0.378363
6	1.867656	3.014070	-0.255989
1	3.913933	2.461551	-0.561836
1	2.032687	4.083745	-0.337636
15	2.025040	-2.002301	0.001127
15	0.273802	2.253602	0.045223
6	-3.986494	-0.961317	-0.165885
1	-4.060917	-2.044577	-0.003555
1	-3.830663	-0.815591	-1.242772
6	2.091034	-3.079932	1.509970
1	1.108943	-3.528448	1.697833
1	2.827341	-3.883936	1.393250
1	2.363815	-2.465188	2.371771
6	1.652093	-3.260155	-1.311658
1	2.401633	-4.060179	-1.320322
1	0.665485	-3.705059	-1.139817
1	1.645621	-2.764290	-2.285942
6	-0.415545	3.056579	1.569995
1	-0.450705	4.147045	1.461555
1	-1.428570	2.689772	1.768701
1	0.220203	2.801450	2.421985
6	-0.877911	2.918951	-1.250803
1	-1.897606	2.556889	-1.077567
1	-0.889589	4.015354	-1.245862
1	-0.546772	2.568802	-2.232187
77	0.865658	0.007702	0.058751

6	-1.471013	-1.045669	0.218690
1	-0.670425	-0.660003	0.950882
1	-1.485371	-2.128202	0.379670
1	-1.235296	-0.861848	-0.837015
6	-5.314781	-0.322923	0.223894
1	-5.510327	-0.467826	1.301840
1	-5.284647	0.767586	0.046984
6	-7.617814	-0.390416	-0.256288
1	-8.335845	-0.910518	-0.896203
1	-7.898166	-0.550980	0.798010
1	-7.672450	0.690974	-0.465048
8	-6.342528	-0.916374	-0.545450
6	-2.797932	-0.391469	0.619498
1	-2.730130	0.691726	0.453761
1	-2.967280	-0.529164	1.696598

Structure 40-41TS - NBE

B3LYP/GBS(1) = -1429.632770 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.940023 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.695972 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.011739 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.056387 a.u.
Enthalpy Correction = 0.416483
Gibbs Free Energy Correction = 0.334068
Imaginary Freq = -742.4 i

Atomic No	x-coord	y-coord	z-coord
7	2.692778	0.749227	-0.283264
6	3.758930	-0.107587	-0.372297
6	3.632620	-1.456192	-0.243543
1	4.735161	0.350350	-0.550566
1	4.492440	-2.114306	-0.320221
6	2.887464	2.104215	-0.362542
6	1.874040	2.999761	-0.224906
1	3.913114	2.437688	-0.539259
1	2.051159	4.068596	-0.294339
15	1.954305	-2.019616	0.052514
15	0.257706	2.267359	0.060368
6	-3.823843	-0.909362	-0.303677
1	-3.839702	-1.995323	-0.142856
1	-3.778360	-0.754332	-1.389625
6	1.987046	-3.054415	1.588764
1	0.995981	-3.483737	1.772343
1	2.715095	-3.869527	1.503780
1	2.254035	-2.419832	2.437749
6	1.581444	-3.297039	-1.238983
1	2.316061	-4.110302	-1.219444
1	0.583771	-3.718694	-1.073814
1	1.599168	-2.821593	-2.223379
6	-0.417334	3.060442	1.593551
1	-0.416808	4.153048	1.505135
1	-1.442151	2.720355	1.776221

1	0.203299	2.768781	2.444847
6	-0.854048	2.987809	-1.239891
1	-1.886699	2.656084	-1.087255
1	-0.829025	4.083596	-1.216367
1	-0.520067	2.644779	-2.222995
77	0.798633	-0.002523	0.054623
6	-1.277138	-0.908753	-0.150001
1	-0.445604	-0.519604	0.975937
1	-1.279815	-1.988357	0.032939
1	-1.198441	-0.755738	-1.233900
6	-5.132052	-0.325135	0.216912
1	-5.217649	-0.484484	1.307058
1	-5.160612	0.766991	0.049221
6	-7.466910	-0.474609	-0.036296
1	-8.226223	-1.016104	-0.607336
1	-7.635879	-0.652089	1.039006
1	-7.581022	0.605689	-0.226972
8	-6.208875	-0.951047	-0.455099
6	-2.586661	-0.296916	0.368734
1	-2.575077	0.787385	0.195651
1	-2.660858	-0.430751	1.457929

Structure 41 - NBE

B3LYP/GBS(1) = -1429.649325 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.954065 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.728069 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.026047 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.067761 a.u.
Enthalpy Correction = 0.417618
Gibbs Free Energy Correction = 0.336346

Atomic No	x-coord	y-coord	z-coord
7	-1.710541	-0.043902	1.540923
6	-2.103646	1.133615	2.096708
6	-1.806337	2.343704	1.537186
1	-2.681640	1.080958	3.024897
1	-2.123902	3.269915	2.007263
6	-2.088602	-1.246955	2.051940
6	-1.781012	-2.432021	1.445415
1	-2.663948	-1.236602	2.983216
1	-2.087472	-3.378675	1.880538
15	-0.870755	2.305499	0.004107
15	-0.858637	-2.320678	-0.091470
6	0.561216	3.458155	0.255381
1	1.106753	3.601123	-0.682951
1	0.211515	4.433542	0.613010
1	1.244276	3.035546	0.998037
6	-1.848731	3.222489	-1.271729
1	-2.074993	4.242766	-0.941756
1	-1.285002	3.265659	-2.209834
1	-2.785420	2.688577	-1.451856
6	0.612655	-3.433501	0.082327

1	0.301780	-4.450429	0.347966
1	1.170341	-3.468831	-0.859379
1	1.272028	-3.048360	0.865063
6	-1.830318	-3.201350	-1.396498
1	-1.273350	-3.197383	-2.339461
1	-2.035321	-4.237944	-1.105967
1	-2.777843	-2.677857	-1.548179
77	-0.585222	-0.005683	-0.309492
6	0.611675	0.036116	-2.054580
1	-1.879623	0.006636	-1.167519
1	0.674657	-0.957865	-2.523054
6	2.040510	0.509156	-1.719922
1	4.009119	1.366381	0.098989
1	4.717253	0.114900	-0.942507
1	2.036175	1.591534	-1.527409
1	2.720520	0.357702	-2.575198
6	2.623452	-0.199351	-0.487207
1	1.961885	-0.043894	0.386791
1	2.659966	-1.282655	-0.655649
8	4.450010	-0.428399	1.043689
6	4.016744	0.280289	-0.104041
6	5.741170	-0.052667	1.463709
1	5.982131	-0.648296	2.348689
1	6.498604	-0.247540	0.686097
1	5.791631	1.016490	1.729780
1	0.193874	0.698307	-2.826424

Structure 42 - NBE

B3LYP/GBS(1) = -1429.624629 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1429.935662 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1428.699695 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.014260 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1430.055746 a.u.
Enthalpy Correction = 0.41337
Gibbs Free Energy Correction = 0.331686

Atomic No	x-coord	y-coord	z-coord
7	2.577770	0.905382	-0.419140
6	2.634236	2.253550	-0.557390
6	1.545562	3.055501	-0.377190
1	3.603079	2.687160	-0.823963
1	1.618614	4.132678	-0.494379
6	3.657838	0.106500	-0.599951
6	3.602413	-1.251128	-0.462930
1	4.600060	0.595824	-0.865699
1	4.484603	-1.865977	-0.613169
15	0.003577	2.246471	0.057565
15	2.010510	-1.946092	-0.025390
6	-1.255574	2.819304	-1.173396
1	-2.247973	2.432749	-0.917060

1	-1.302534	3.914067	-1.206366
1	-0.977240	2.439225	-2.159349
6	-0.597520	3.059228	1.609036
1	-0.689122	4.143426	1.475677
1	-1.573108	2.655209	1.900497
1	0.118076	2.851865	2.408369
6	1.594203	-3.241172	-1.278539
1	2.373257	-4.010505	-1.328907
1	0.642582	-3.719829	-1.021865
1	1.491277	-2.762910	-2.255497
6	2.239063	-2.965722	1.500827
1	1.291225	-3.438239	1.781762
1	2.992200	-3.747570	1.349361
1	2.554943	-2.308325	2.314455
77	0.672221	-0.018780	0.102493
6	-2.328479	-0.372966	0.823461
6	-0.947528	-0.892295	0.537230
1	-2.578339	-0.658847	1.860324
1	-2.365727	0.719991	0.777700
1	-0.967731	-1.992742	0.606209
6	-4.800126	-0.512732	0.226332
1	-4.867327	0.588592	0.162255
1	-5.053783	-0.789839	1.265747
1	1.251130	0.253143	1.647547
1	0.528421	-0.042670	-1.563375
6	-7.043500	-0.727853	-0.448239
1	-7.181099	0.360680	-0.557976
1	-7.660098	-1.239190	-1.192354
1	-7.386381	-1.017369	0.559019
6	-3.389902	-0.980027	-0.117623
8	-5.706651	-1.112177	-0.677566
1	-3.166562	-0.706095	-1.155363
1	-3.360057	-2.075504	-0.063451

Structure 44 - NBE

B3LYP/GBS(1) = -1428.431002 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1428.730401 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1427.496732 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1428.804093 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1428.847121 a.u.
Enthalpy Correction = 0.397144
Gibbs Free Energy Correction = 0.315407

Atomic No	x-coord	y-coord	z-coord
7	2.530285	0.896092	-0.418464
6	3.637030	0.108452	-0.617679
6	3.606020	-1.244996	-0.483072
1	4.564623	0.618682	-0.894025
1	4.494671	-1.847640	-0.643756
6	2.598876	2.259488	-0.571783
6	1.520199	3.066291	-0.392855
1	3.570524	2.679171	-0.848927

1	1.595054	4.142335	-0.518238
15	2.006885	-1.933709	-0.024397
15	-0.012813	2.230057	0.061685
6	2.285761	-2.970561	1.485260
1	1.349585	-3.454564	1.783285
1	3.041964	-3.742674	1.302749
1	2.619054	-2.326027	2.302912
6	1.590488	-3.221060	-1.288835
1	2.376604	-3.981607	-1.357002
1	0.646458	-3.709748	-1.025130
1	1.470190	-2.737293	-2.261570
6	-0.594776	3.071178	1.608857
1	-0.691504	4.152365	1.456641
1	-1.564645	2.667535	1.917945
1	0.129054	2.885200	2.406798
6	-1.272526	2.805913	-1.171311
1	-2.265514	2.426709	-0.908088
1	-1.311173	3.900661	-1.211128
1	-1.004206	2.420049	-2.158358
77	0.693845	-0.010091	0.112132
6	-0.921138	-0.892138	0.550428
6	-2.311466	-0.388940	0.840802
1	-2.567631	-0.684420	1.874569
1	-2.361233	0.704986	0.806127
1	-5.045081	-0.821888	1.259470
1	-4.853421	0.569358	0.173406
6	-3.367753	-0.990904	-0.109701
1	-3.333209	-2.086698	-0.063463
1	-3.139418	-0.709809	-1.144843
6	-4.782420	-0.532464	0.225692
8	-5.681911	-1.123509	-0.692581
6	-7.020842	-0.747356	-0.466141
1	-7.162407	0.342247	-0.561550
1	-7.631893	-1.250439	-1.220645
1	-7.369166	-1.051445	0.535127
1	-0.955863	-1.995225	0.616135

2.5. Coordinates of NBE structures at the Full-opt level of theory

Full Structure 3 - NBE

B3LYP/GBS(1) = -2130.045853 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2130.541704 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2129.370491 a.u.
Enthalpy Correction = 0.819491
Gibbs Free Energy Correction = 0.691159

Atomic No	x-coord	y-coord	z-coord
8	-3.278917	-1.590145	0.340292
6	-4.307173	-2.241108	-0.395415
1	-4.223551	-3.334291	-0.268059

1	-4.192300	-2.029147	-1.472344
77	-0.030938	-0.375461	0.051083
6	-1.990531	-2.008553	-0.052984
1	-1.289841	-1.539972	0.743362
1	-1.847464	-3.088557	0.103799
1	-1.775850	-1.772678	-1.103300
6	-5.659591	-1.752508	0.107227
1	-5.720579	-1.941770	1.186956
1	-5.714144	-0.663511	-0.024407
6	-6.836634	-2.424705	-0.611915
1	-6.771585	-3.513940	-0.479223
1	-6.757044	-2.243384	-1.693160
6	-8.198685	-1.931568	-0.112086
1	-9.020253	-2.428505	-0.640087
1	-8.321993	-2.128974	0.959694
1	-8.308707	-0.850981	-0.264540
15	-1.254209	1.549287	0.446602
6	-0.030796	2.803990	-0.050720
6	-2.803505	1.770740	-0.605683
6	-1.771837	1.992356	2.198001
6	-0.299913	4.168810	-0.224924
6	1.257770	2.279013	-0.343663
6	-2.434891	1.699917	-2.097081
6	-3.690361	2.991164	-0.312379
1	-3.371396	0.865355	-0.355127
1	-2.176491	3.013417	2.160694
6	-0.541269	1.989216	3.118276
6	-2.859188	1.042201	2.723224
6	0.638081	5.055236	-0.756003
1	-1.277325	4.553446	0.054333
6	2.177389	3.167852	-0.955393
7	1.528533	0.931764	-0.086704
1	-1.861489	2.580945	-2.405674
1	-3.345292	1.658863	-2.709054
1	-1.828278	0.814140	-2.313712
1	-3.200858	3.927466	-0.598764
1	-4.615480	2.920079	-0.899627
1	-3.978459	3.063342	0.741202
1	0.214305	2.707161	2.784385
1	-0.836280	2.254689	4.141599
1	-0.075827	0.997592	3.137218
1	-3.765346	1.056942	2.109152
1	-3.141904	1.326851	3.744819
1	-2.495815	0.009342	2.747846
6	0.339225	6.526044	-0.926989
6	1.870654	4.507398	-1.148174
1	3.133285	2.793241	-1.301331
6	2.827359	0.462552	0.107545
1	0.539136	6.865233	-1.951692
1	-0.710177	6.747419	-0.704079
1	0.953179	7.147236	-0.260642
1	2.609916	5.147045	-1.627698
6	3.914653	1.275490	0.520023
6	3.103003	-0.925402	-0.046256
1	3.740925	2.315983	0.766074
6	5.197873	0.762785	0.640891
6	4.417086	-1.407145	0.044964
15	1.626484	-1.962365	-0.279117
1	5.995663	1.429398	0.964654
6	5.495322	-0.583403	0.368973
1	4.605538	-2.462328	-0.136017

6	1.868029	-2.821094	-1.935973
6	1.662337	-3.353578	0.997997
6	6.908832	-1.109773	0.448806
6	1.959095	-1.770871	-3.053836
1	2.826077	-3.355858	-1.880588
6	0.750352	-3.835022	-2.222971
6	2.746085	-4.432564	0.842015
1	0.684366	-3.835298	0.849638
6	1.679505	-2.758039	2.415977
1	7.536139	-0.721000	-0.365159
1	7.395899	-0.823623	1.389847
1	6.931451	-2.203119	0.383529
1	2.121555	-2.262243	-4.021764
1	2.783965	-1.072335	-2.883435
1	1.033668	-1.186788	-3.112883
1	0.921766	-4.322055	-3.191133
1	-0.224735	-3.336325	-2.274122
1	0.688936	-4.622898	-1.464363
1	2.763233	-4.881684	-0.156519
1	3.741912	-4.031451	1.054236
1	2.563493	-5.241051	1.561741
1	2.631784	-2.255139	2.617652
1	0.878602	-2.022792	2.545617
1	1.553711	-3.554574	3.160547

Full Structure 3-5TS - NBE

B3LYP/GBS(1) = -2130.043894 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2130.542361 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2129.371597 a.u.
Enthalpy Correction = 0.816223
Gibbs Free Energy Correction = 0.691487
Imaginary Freq = -585.1 i

Atomic No	x-coord	y-coord	z-coord
8	3.215208	-1.341198	0.998380
6	3.813700	-2.196653	0.035692
1	3.328926	-2.057163	-0.945567
1	3.657303	-3.249303	0.328381
77	0.128390	-0.326868	0.238659
6	1.839118	-1.582101	1.194601
1	1.369760	-1.391546	-0.078433
1	1.645932	-2.659144	1.278727
1	1.562421	-1.093266	2.129468
6	5.302584	-1.888304	-0.051910
1	5.429514	-0.834736	-0.333208
1	5.743682	-2.002143	0.947190
6	6.034951	-2.788321	-1.055942
1	5.573306	-2.680623	-2.047699
1	5.900108	-3.840910	-0.769231
6	7.531856	-2.476222	-1.155182
1	8.028793	-3.134478	-1.876699
1	7.700017	-1.441116	-1.476575

1	8.028910	-2.606706	-0.186195
15	-1.515630	-1.955987	0.413158
6	-2.953465	-1.030834	-0.217834
6	-1.238924	-3.459427	-0.694071
6	-2.079522	-2.660933	2.065473
6	-4.200983	-1.600363	-0.510239
6	-2.712750	0.351978	-0.455870
6	-1.020319	-3.002225	-2.146327
6	-2.276977	-4.590316	-0.622301
1	-0.282528	-3.854336	-0.321207
1	-2.983336	-3.250636	1.859449
6	-2.455426	-1.517805	3.021390
6	-1.022997	-3.580660	2.697009
6	-5.229391	-0.878930	-1.118469
1	-4.376977	-2.644102	-0.261864
6	-3.733884	1.054254	-1.145756
7	-1.493854	0.910572	-0.069047
1	-1.944267	-2.595839	-2.572257
1	-0.708580	-3.853418	-2.765186
1	-0.252661	-2.223723	-2.202752
1	-3.236888	-4.279950	-1.046201
1	-1.925503	-5.446820	-1.212001
1	-2.452015	-4.946028	0.398200
1	-3.241344	-0.882954	2.601402
1	-2.818784	-1.927257	3.972596
1	-1.588013	-0.881843	3.231251
1	-0.758483	-4.426639	2.053107
1	-1.399672	-3.991916	3.641940
1	-0.104551	-3.027247	2.923089
6	-6.575601	-1.498485	-1.410956
6	-4.944160	0.452671	-1.460898
1	-3.564102	2.078655	-1.454194
6	-1.324514	2.292302	0.069159
1	-6.903759	-1.289533	-2.437040
1	-6.549678	-2.586628	-1.286404
1	-7.357135	-1.112392	-0.741918
1	-5.691588	1.036808	-1.995538
6	-2.368275	3.192090	0.399153
6	-0.022611	2.851202	-0.050486
1	-3.358676	2.806147	0.609383
6	-2.146009	4.559619	0.488283
6	0.166049	4.238666	0.009460
15	1.321478	1.622020	-0.176893
1	-2.980978	5.207271	0.750895
6	-0.881795	5.126393	0.261020
1	1.165135	4.642478	-0.133177
6	2.108606	1.916763	-1.857759
6	2.645205	2.059220	1.092753
6	-0.667200	6.620807	0.311073
6	1.057363	1.758248	-2.966968
1	2.461311	2.957392	-1.858159
6	3.304546	0.984464	-2.097423
6	3.556606	3.257598	0.782728
1	3.259197	1.149338	1.098854
6	2.005223	2.202184	2.484502
1	-1.139918	7.129893	-0.540064
1	-1.092622	7.061758	1.221627
1	0.399028	6.871366	0.289095
1	1.516296	1.939276	-3.947462
1	0.230322	2.463727	-2.843141
1	0.639216	0.745748	-2.961975

1	3.762860	1.202526	-3.070395
1	2.977983	-0.061081	-2.107237
1	4.081096	1.088993	-1.332219
1	4.035237	3.185405	-0.198999
1	3.013051	4.206968	0.828339
1	4.356777	3.309213	1.532576
1	1.391015	3.107020	2.547197
1	1.362961	1.347460	2.721219
1	2.787394	2.268685	3.251114

Full Structure 5 - NBE

B3LYP/GBS(1) = -2130.065782 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2130.563690 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2129.388730 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -2125.371669 a.u.
Enthalpy Correction = 0.817404
Gibbs Free Energy Correction = 0.690887

Atomic No	x-coord	y-coord	z-coord
8	2.937581	-1.362983	-0.107553
6	3.927340	-2.277659	-0.538174
1	3.985692	-2.291791	-1.642598
1	3.659783	-3.302174	-0.222572
6	1.618777	-1.708469	-0.564259
1	1.425961	-2.750200	-0.257096
1	1.621252	-1.697562	-1.673256
77	0.106522	-0.383982	0.044444
1	0.885281	-0.882005	1.309270
6	5.275447	-1.883681	0.056801
1	5.517979	-0.860557	-0.261839
1	5.178871	-1.856420	1.150661
6	6.409966	-2.835272	-0.343922
1	6.153471	-3.858617	-0.034721
1	6.496163	-2.861080	-1.439538
6	7.761761	-2.445326	0.263662
1	8.552267	-3.141858	-0.038637
1	8.063820	-1.439658	-0.053976
1	7.717561	-2.445787	1.359755
15	-1.588765	-1.933298	0.391205
6	-3.063221	-0.920547	0.001817
6	-1.589164	-3.411429	-0.778355
6	-1.848731	-2.640811	2.106165
6	-4.363585	-1.434548	-0.096213
6	-2.798002	0.442051	-0.319449
6	-1.633033	-2.923411	-2.236374
6	-2.638920	-4.506965	-0.533329
1	-0.595913	-3.846946	-0.602371
1	-2.783295	-3.217221	2.070389
6	-2.017599	-1.507656	3.130334
6	-0.696398	-3.580851	2.496580
6	-5.432815	-0.681541	-0.587211
1	-4.550507	-2.460801	0.209622

6	-3.866442	1.165988	-0.902140
7	-1.508468	0.956890	-0.121144
1	-2.597542	-2.458972	-2.468327
1	-1.492756	-3.770548	-2.919162
1	-0.845791	-2.190047	-2.438443
1	-3.648472	-4.157589	-0.771468
1	-2.430568	-5.362923	-1.187988
1	-2.637533	-4.876402	0.497229
1	-2.860880	-0.857298	2.877852
1	-2.198971	-1.930169	4.126646
1	-1.116672	-0.887121	3.179300
1	-0.601314	-4.434397	1.816280
1	-0.864366	-3.979446	3.504782
1	0.258964	-3.044471	2.500382
6	-6.833362	-1.242002	-0.665439
6	-5.136963	0.617552	-1.025980
1	-3.689186	2.166639	-1.277874
6	-1.270496	2.325151	0.087928
1	-7.288998	-1.057786	-1.646362
1	-6.840632	-2.323877	-0.493795
1	-7.495592	-0.788117	0.084500
1	-5.922508	1.218903	-1.480605
6	-2.257524	3.261897	0.477404
6	0.062341	2.820041	-0.006028
1	-3.266069	2.924518	0.680649
6	-1.962316	4.610999	0.638559
6	0.322041	4.190255	0.121676
15	1.377536	1.556765	-0.210875
1	-2.761053	5.285743	0.942086
6	-0.675130	5.121214	0.425273
1	1.340177	4.548006	-0.007289
6	2.146869	1.981487	-1.875034
6	2.707409	1.848155	1.085524
6	-0.378988	6.598629	0.531981
6	1.091357	1.845061	-2.985132
1	2.434510	3.040063	-1.805840
6	3.396562	1.150231	-2.201828
6	3.617623	3.071681	0.892707
1	3.308473	0.937044	0.978006
6	2.087993	1.848589	2.492976
1	-0.704213	7.145478	-0.364039
1	-0.893687	7.052849	1.387365
1	0.694101	6.783529	0.652812
1	1.518490	2.157012	-3.946573
1	0.210354	2.463687	-2.789072
1	0.760083	0.805194	-3.085757
1	3.804192	1.469139	-3.169745
1	3.157340	0.085572	-2.263945
1	4.185628	1.264332	-1.452288
1	4.056008	3.127230	-0.108288
1	3.084138	4.008109	1.085414
1	4.446442	3.020666	1.610375
1	1.446622	2.724088	2.643885
1	1.486657	0.951774	2.667103
1	2.884345	1.879612	3.247267

Full Structure 6 – 8TS - NBE

B3LYP/GBS(1) = -2130.005486 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2130.511010 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2129.333434 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -2125.346370 a.u.
Enthalpy Correction = 0.809969
Gibbs Free Energy Correction = 0.684748
Imaginary Freq = -963.6 i

Atomic No	x-coord	y-coord	z-coord
8	3.041704	-0.874578	-0.311127
6	4.032854	-1.830121	-0.724969
1	3.971024	-1.957746	-1.815513
1	3.814332	-2.798041	-0.256121
6	1.764135	-1.299822	-0.143202
1	1.740069	-2.396910	-0.241120
77	0.276930	-0.245286	0.443214
1	0.644617	-0.137546	2.051115
1	-0.297755	0.407363	2.001870
6	5.407407	-1.308473	-0.323387
1	5.524223	-0.300943	-0.741633
1	5.438481	-1.202230	0.769277
6	6.568332	-2.197548	-0.799770
1	7.509271	-1.675415	-0.584446
1	6.523533	-2.300123	-1.893402
6	6.611693	-3.589257	-0.154869
1	7.496833	-4.145316	-0.483488
1	6.651810	-3.515448	0.938999
1	5.733406	-4.191567	-0.414392
15	-1.227918	-2.049158	0.551368
6	-2.701433	-1.328272	-0.250730
6	-0.754892	-3.614403	-0.403757
6	-1.804226	-2.690434	2.226660
6	-3.840605	-2.087940	-0.567343
6	-2.646717	0.060135	-0.575480
6	-0.658650	-3.307652	-1.907532
6	-1.592468	-4.880934	-0.157948
1	0.259847	-3.825441	-0.037746
1	-2.545559	-3.471857	2.013370
6	-2.500132	-1.593281	3.044743
6	-0.636497	-3.312244	3.009809
6	-4.927019	-1.562719	-1.264284
1	-3.881318	-3.130137	-0.261687
6	-3.732657	0.565589	-1.344232
7	-1.549599	0.809666	-0.209534
1	-1.651481	-3.132406	-2.334936
1	-0.207020	-4.157499	-2.435048
1	-0.050807	-2.418020	-2.095637
1	-2.615619	-4.773293	-0.530847
1	-1.140550	-5.721987	-0.699598
1	-1.640817	-5.163289	0.897938
1	-3.360183	-1.177318	2.511704
1	-2.855953	-2.011243	3.995040
1	-1.814891	-0.770072	3.271984
1	-0.153202	-4.131809	2.465922
1	-0.995177	-3.715930	3.964916
1	0.129065	-2.559453	3.228871
6	-6.146546	-2.392949	-1.588570
6	-4.824940	-0.220259	-1.671314

1	-3.690634	1.585668	-1.707776
6	-1.573188	2.181270	-0.022515
1	-6.372234	-2.382504	-2.663038
1	-6.007580	-3.438131	-1.291048
1	-7.042527	-2.022210	-1.072219
1	-5.623296	0.217345	-2.268892
6	-2.742450	2.948431	0.218390
6	-0.333983	2.888626	0.020616
1	-3.701085	2.448855	0.290327
6	-2.685330	4.321581	0.411732
6	-0.312729	4.279418	0.187263
15	1.159897	1.848468	-0.166769
1	-3.612041	4.858922	0.607675
6	-1.474488	5.030612	0.377039
1	0.640715	4.799696	0.183160
6	1.649757	2.159097	-1.964623
6	2.588715	2.534044	0.856329
6	-1.432881	6.530334	0.554578
6	0.496742	1.778762	-2.907446
1	1.790092	3.247999	-2.020829
6	2.949240	1.470212	-2.403777
6	3.290057	3.801182	0.334415
1	3.304526	1.703116	0.796061
6	2.189332	2.702779	2.331216
1	-1.973938	6.848543	1.455137
1	-0.402662	6.892166	0.643931
1	-1.891272	7.056204	-0.294247
1	0.786361	1.987583	-3.945332
1	-0.412361	2.344943	-2.688352
1	0.258816	0.713519	-2.822437
1	3.210947	1.799525	-3.417633
1	2.823064	0.385427	-2.419542
1	3.796728	1.696646	-1.749117
1	3.590006	3.723287	-0.714096
1	2.664398	4.692661	0.441841
1	4.199652	3.976417	0.923265
1	1.425255	3.478093	2.452523
1	1.797349	1.773722	2.752681
1	3.067203	2.997966	2.919556

Full Structure 8 - NBE

B3LYP/GBS(1) = -2128.871389 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2129.362628 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2128.192560 a.u.
Enthalpy Correction = 0.797145
Gibbs Free Energy Correction = 0.672396

Atomic No	x-coord	y-coord	z-coord
77	0.148684	-0.375829	0.005283
8	2.924916	-1.275710	-0.049578
6	3.862043	-2.363713	-0.155614
1	3.746920	-2.840990	-1.138784
1	3.634269	-3.113021	0.614983

6	1.601656	-1.582124	-0.042050
1	1.500705	-2.682368	-0.083333
6	5.271712	-1.817901	0.019143
1	5.445494	-1.039751	-0.735584
1	5.342323	-1.328273	0.999491
6	6.343930	-2.909544	-0.099814
1	6.156580	-3.690120	0.651107
1	6.258016	-3.400738	-1.079325
6	7.766136	-2.366320	0.074649
1	8.510351	-3.165759	-0.012259
1	7.997141	-1.610394	-0.685663
1	7.892732	-1.897156	1.057863
15	-1.505580	-1.975880	0.325230
6	-3.009726	-0.992690	-0.009485
6	-1.464944	-3.426573	-0.878537
6	-1.758071	-2.742844	2.020642
6	-4.292884	-1.541032	-0.136783
6	-2.790755	0.399808	-0.220617
6	-1.496274	-2.904389	-2.324690
6	-2.490724	-4.552866	-0.673910
1	-0.465462	-3.849445	-0.700218
1	-2.682499	-3.334529	1.972190
6	-1.942278	-1.636999	3.071507
6	-0.588900	-3.668813	2.392591
6	-5.392845	-0.787708	-0.553775
1	-4.442481	-2.593890	0.087981
6	-3.893683	1.133760	-0.723922
7	-1.515130	0.928944	0.000215
1	-2.467863	-2.455987	-2.559557
1	-1.327536	-3.731453	-3.026120
1	-0.725085	-2.144652	-2.486617
1	-3.504252	-4.222089	-0.920780
1	-2.252587	-5.389213	-1.343890
1	-2.497460	-4.944582	0.348495
1	-2.800307	-0.998932	2.838548
1	-2.106601	-2.082671	4.060891
1	-1.052927	-0.999250	3.123602
1	-0.467684	-4.498687	1.687190
1	-0.753618	-4.103050	3.386763
1	0.351727	-3.107189	2.422644
6	-6.774671	-1.387609	-0.665569
6	-5.145965	0.553706	-0.881566
1	-3.757132	2.167731	-1.016308
6	-1.302091	2.297640	0.204585
1	-7.260232	-1.111659	-1.609957
1	-6.740263	-2.481603	-0.617403
1	-7.434925	-1.046639	0.143977
1	-5.956948	1.164258	-1.275574
6	-2.281720	3.201236	0.685327
6	0.001098	2.835213	-0.002010
1	-3.256279	2.827335	0.975178
6	-2.018703	4.558604	0.822095
6	0.224979	4.214410	0.102389
15	1.327665	1.606470	-0.297748
1	-2.808114	5.207568	1.198016
6	-0.772293	5.111090	0.494207
1	1.213925	4.606959	-0.119170
6	2.048121	2.071099	-1.969987
6	2.696723	1.920455	0.957321
6	-0.518566	6.597876	0.578094
6	0.971300	1.936392	-3.058287

1	2.337584	3.128963	-1.899045
6	3.291310	1.239396	-2.320270
6	3.502842	3.220216	0.815638
1	3.365270	1.072136	0.767457
6	2.136335	1.765503	2.380683
1	-0.988522	7.140298	-0.254140
1	-0.921094	7.025822	1.504699
1	0.553356	6.822380	0.547231
1	1.378381	2.248894	-4.028547
1	0.095952	2.556546	-2.841797
1	0.635265	0.897249	-3.144810
1	3.675135	1.541254	-3.303181
1	3.047037	0.173266	-2.361177
1	4.099762	1.368631	-1.592809
1	3.886915	3.374661	-0.198184
1	2.908210	4.095749	1.094192
1	4.367148	3.188995	1.491918
1	1.432670	2.571235	2.619003
1	1.611385	0.811227	2.492669
1	2.953712	1.804318	3.112371

Structure 10 - NBE

B3LYP/GBS(1) = -2130.041966 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2130.533936 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2129.371277 a.u.
Enthalpy Correction = 0.820077
Gibbs Free Energy Correction = 0.695287

Atomic No	x-coord	y-coord	z-coord
8	0.884183	-3.624593	1.608598
77	-0.012770	-0.451916	0.178736
6	-0.089508	-3.379561	0.638055
6	0.004769	-4.444693	-0.450453
1	0.098875	-2.377312	0.105785
1	-1.095531	-3.342820	1.074723
1	1.024155	-4.438497	-0.855372
1	-0.135144	-5.420699	0.033427
6	0.661733	-2.923025	2.823124
1	-0.234748	-3.302265	3.336995
1	0.538487	-1.847369	2.622782
6	-1.014426	-4.262633	-1.579752
1	-2.030825	-4.281143	-1.161242
1	-0.886122	-3.268843	-2.027835
6	-0.892343	-5.338778	-2.664253
1	-1.632787	-5.187723	-3.457598
1	0.101442	-5.321853	-3.127991
1	-1.047079	-6.342166	-2.248875
1	1.536270	-3.092240	3.455543
15	2.245173	-0.306680	-0.318049
6	2.487804	1.490214	-0.150085
6	3.442966	-1.162864	0.870098
6	2.859055	-0.737043	-2.044051
6	3.730513	2.138031	-0.123995

6	1.286442	2.223389	0.045948
6	3.369500	-0.493536	2.253743
6	4.903729	-1.313164	0.414525
1	3.008874	-2.167786	0.959736
1	3.927096	-0.482146	-2.073542
6	2.124674	0.110861	-3.093915
6	2.693429	-2.234716	-2.341825
6	3.859612	3.497859	0.162298
1	4.630693	1.560769	-0.321240
6	1.430157	3.584919	0.414281
7	0.054508	1.572024	-0.060943
1	3.857206	0.486664	2.243616
1	3.878283	-1.117624	2.999561
1	2.333927	-0.344776	2.574852
1	5.405643	-0.344625	0.316517
1	5.460708	-1.889706	1.164608
1	4.999041	-1.842685	-0.538379
1	2.292090	1.180843	-2.938262
1	2.478850	-0.147463	-4.100269
1	1.044969	-0.070379	-3.050361
1	3.194781	-2.873434	-1.605932
1	3.111106	-2.473569	-3.328104
1	1.631159	-2.501795	-2.354610
6	5.202903	4.188585	0.170188
6	2.676605	4.192751	0.464152
1	0.553277	4.161705	0.682771
6	-1.122049	2.261161	-0.354620
1	5.344555	4.789230	1.077650
1	6.023898	3.464994	0.120003
1	5.316303	4.870449	-0.683935
1	2.733935	5.239708	0.757591
6	-1.162866	3.518431	-1.011233
6	-2.377852	1.668691	-0.047204
1	-0.243570	3.962626	-1.373296
6	-2.360053	4.187165	-1.220056
6	-3.568617	2.385088	-0.236541
15	-2.278965	-0.068156	0.489778
1	-2.336781	5.148659	-1.730567
6	-3.594022	3.659751	-0.803351
1	-4.510932	1.931701	0.060989
6	-3.117683	-0.102154	2.174700
6	-3.413263	-1.072861	-0.641672
6	-4.881202	4.429416	-0.982666
6	-2.351878	0.799057	3.155703
1	-4.122611	0.317415	2.030959
6	-3.255153	-1.527972	2.729298
6	-4.930565	-0.893245	-0.474764
1	-3.165017	-2.108924	-0.370753
6	-2.996193	-0.857582	-2.106164
1	-4.946939	5.282210	-0.292888
1	-4.973574	4.834375	-1.998512
1	-5.754665	3.794307	-0.798561
1	-2.846553	0.797379	4.135604
1	-2.305514	1.832641	2.799554
1	-1.323190	0.444877	3.287016
1	-3.792838	-1.510334	3.685772
1	-2.270501	-1.971039	2.914929
1	-3.805109	-2.194056	2.055339
1	-5.270793	-1.051616	0.553519
1	-5.253763	0.102686	-0.792900
1	-5.455763	-1.619886	-1.108359

1	-3.254497	0.153276	-2.440246
1	-1.916117	-0.986107	-2.231616
1	-3.516817	-1.572220	-2.756465

Full Structure 10-11TS - NBE

B3LYP/GBS(1) = -2130.030701 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2130.527839 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2129.366227 a.u.
Enthalpy Correction = 0.816039
Gibbs Free Energy Correction = 0.692482
Imaginary Freq = -704.7 i

Atomic No	x-coord	y-coord	z-coord
8	0.897044	-2.960965	1.780539
77	-0.026238	-0.535110	0.162684
6	-0.126765	-2.828660	0.823460
6	-0.045850	-4.104991	-0.039657
1	-0.106778	-2.061865	-0.394510
1	-1.107890	-2.792743	1.303100
1	0.926971	-4.128834	-0.549269
1	-0.052056	-4.954697	0.656628
6	0.624138	-2.351390	3.031636
1	-0.277428	-2.785235	3.492281
1	0.486262	-1.268960	2.920539
6	-1.174113	-4.269467	-1.063307
1	-2.142954	-4.244552	-0.543554
1	-1.175828	-3.417878	-1.756374
6	-1.060431	-5.574172	-1.860447
1	-1.878574	-5.671845	-2.583020
1	-0.116590	-5.615501	-2.417681
1	-1.092343	-6.448549	-1.198988
1	1.482682	-2.555358	3.676298
15	-2.304907	-0.070019	0.352135
6	-2.301378	1.712548	-0.032930
6	-3.369626	-0.929559	-0.953509
6	-3.324131	-0.185481	1.936052
6	-3.458657	2.482815	-0.217799
6	-1.012119	2.287745	-0.209487
6	-2.778652	-0.682157	-2.351452
6	-4.878004	-0.632203	-0.944670
1	-3.230549	-1.993051	-0.714835
1	-4.272623	0.322101	1.714387
6	-2.630159	0.579585	3.073468
6	-3.634430	-1.631722	2.350212
6	-3.417036	3.804568	-0.663387
1	-4.428816	2.035733	-0.016530
6	-0.983036	3.601813	-0.744395
7	0.121038	1.527297	0.083174
1	-2.880977	0.370416	-2.638359
1	-3.308844	-1.288739	-3.096943
1	-1.714619	-0.936162	-2.379856
1	-5.083489	0.393431	-1.266244

1	-5.383877	-1.300384	-1.653579
1	-5.343130	-0.784013	0.034868
1	-2.450998	1.625006	2.804910
1	-3.255900	0.562240	3.975081
1	-1.664251	0.126546	3.322364
1	-4.144593	-2.198532	1.563928
1	-4.284344	-1.637020	3.234412
1	-2.719836	-2.172765	2.616491
6	-4.670383	4.628653	-0.841321
6	-2.147262	4.325901	-0.958738
1	-0.034127	4.051902	-1.008614
6	1.386149	2.120251	0.203365
1	-4.692256	5.127725	-1.818496
1	-5.570066	4.007955	-0.766564
1	-4.753561	5.416404	-0.079796
1	-2.066339	5.329932	-1.372404
6	1.601369	3.429859	0.696187
6	2.544580	1.362296	-0.112032
1	0.757899	4.010851	1.050572
6	2.874977	3.980349	0.759337
6	3.814362	1.952566	-0.070444
15	2.219960	-0.406710	-0.433272
1	2.988858	4.989687	1.151342
6	4.013083	3.271201	0.344972
1	4.681812	1.362679	-0.355618
6	2.603391	-0.676524	-2.256119
6	3.529769	-1.405990	0.498753
6	5.386181	3.900528	0.369765
6	1.819512	0.313892	-3.130630
1	3.675454	-0.475222	-2.384829
6	2.312934	-2.126484	-2.675186
6	4.896463	-1.581997	-0.184131
1	3.055780	-2.391083	0.579829
6	3.702812	-0.865996	1.928385
1	5.584651	4.402299	1.325211
1	6.171207	3.151530	0.219011
1	5.501616	4.657587	-0.418038
1	2.053137	0.141293	-4.189212
1	2.072678	1.351216	-2.891888
1	0.740488	0.190396	-2.990834
1	2.586898	-2.277859	-3.726973
1	1.245055	-2.347365	-2.568798
1	2.869351	-2.859096	-2.079584
1	4.821817	-2.047482	-1.171256
1	5.429916	-0.632253	-0.298256
1	5.527380	-2.232454	0.435587
1	4.254263	0.079610	1.935006
1	2.740097	-0.692404	2.415152
1	4.264179	-1.590232	2.532037

Full Structure 11-13TS - NBE

B3LYP/GBS(1) = -2130.019566 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2130.523311 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2129.359404 a.u.

Enthalpy Correction = 0.813036
Gibbs Free Energy Correction = 0.694242
Imaginary Freq = -782.9 i

Atomic No	x-coord	y-coord	z-coord
8	1.439951	-3.415890	0.364020
77	0.006332	-0.663539	0.054313
6	0.184407	-2.800772	0.200226
6	-0.237621	-2.586285	-1.170672
1	0.240209	-0.296449	1.627436
1	-0.559388	-3.240838	0.870318
6	1.707210	-3.770576	1.705230
1	0.966727	-4.493621	2.083193
1	1.704390	-2.892017	2.364771
1	-0.248958	-0.996581	-1.613539
1	-1.303591	-2.719402	-1.316495
6	0.542435	-3.119236	-2.360781
1	0.183394	-2.634918	-3.277517
1	1.600392	-2.879168	-2.269696
6	0.372468	-4.643193	-2.474012
1	-0.683379	-4.922845	-2.577648
1	0.905140	-5.025363	-3.352476
1	0.773918	-5.140224	-1.585856
1	2.695507	-4.238098	1.724295
15	-2.275661	-0.488497	0.579159
6	-2.671922	1.157350	-0.089934
6	-3.485702	-1.728996	-0.194728
6	-2.747938	-0.451914	2.398540
6	-3.979308	1.631429	-0.280340
6	-1.549143	1.943985	-0.473166
6	-3.640290	-1.474102	-1.705887
6	-4.867612	-1.872502	0.468201
1	-2.971703	-2.691446	-0.060899
1	-3.840064	-0.342221	2.418088
6	-2.139996	0.761072	3.117100
6	-2.361269	-1.763343	3.100614
6	-4.251297	2.843114	-0.913631
1	-4.816482	1.030714	0.065980
6	-1.841140	3.140889	-1.183162
7	-0.271397	1.483127	-0.210693
1	-4.267273	-0.596964	-1.890521
1	-4.117597	-2.339366	-2.182694
1	-2.681796	-1.293372	-2.201106
1	-5.454929	-0.950865	0.405601
1	-5.436155	-2.653220	-0.053251
1	-4.805071	-2.163732	1.520433
1	-2.462237	1.702458	2.662311
1	-2.458558	0.762490	4.167306
1	-1.046428	0.727624	3.090475
1	-2.811936	-2.644987	2.629798
1	-2.692827	-1.742713	4.146274
1	-1.274063	-1.894151	3.091954
6	-5.662385	3.347268	-1.103389
6	-3.143591	3.565999	-1.390965
1	-1.025620	3.721122	-1.598238
6	0.812832	2.319749	-0.058375
1	-5.862533	3.610025	-2.150198
1	-6.398705	2.592705	-0.805572
1	-5.857908	4.248430	-0.506268

1	-3.309192	4.484758	-1.951511
6	0.717966	3.715616	0.209813
6	2.132042	1.781286	-0.097345
1	-0.255444	4.157190	0.385030
6	1.838466	4.525896	0.273599
6	3.246022	2.638902	-0.074600
15	2.292872	-0.038701	-0.104973
1	1.704402	5.586867	0.479527
6	3.136046	4.018436	0.086141
1	4.240412	2.214989	-0.179253
6	3.410189	-0.378811	-1.588844
6	3.408934	-0.504504	1.359616
6	4.345018	4.923772	0.085187
6	2.677700	-0.059836	-2.900984
1	4.226050	0.349278	-1.493535
6	4.030777	-1.788108	-1.579062
6	4.858741	0.017635	1.312844
1	3.437493	-1.599095	1.289181
6	2.796842	-0.118678	2.715118
1	4.382482	5.556060	-0.812796
1	4.346397	5.600200	0.949726
1	5.275756	4.346530	0.115494
1	3.370085	-0.160294	-3.746502
1	2.290588	0.964088	-2.899958
1	1.833898	-0.733247	-3.071596
1	4.505462	-1.994770	-2.546548
1	3.290935	-2.569174	-1.387976
1	4.802453	-1.886631	-0.809357
1	5.357187	-0.129901	0.350887
1	4.898757	1.083058	1.557282
1	5.451850	-0.509440	2.071053
1	2.669728	0.967383	2.790764
1	1.820887	-0.579498	2.873738
1	3.468528	-0.434868	3.523827

Structure 16 - NBE

B3LYP/GBS(1) = -2128.860178 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2129.349592 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2128.191722 a.u.
Enthalpy Correction = 0.796892
Gibbs Free Energy Correction = 0.673381

Atomic No	x-coord	y-coord	z-coord
8	0.273969	-3.222853	1.522583
77	0.000031	-0.603495	0.178310
6	-0.041931	-2.509162	0.424607
6	-0.528856	-3.526176	-0.604952
1	-1.510068	-3.892027	-0.261203
1	-0.698942	-3.003386	-1.550163
6	0.680858	-2.556162	2.725410
1	0.480076	-1.484773	2.636290
1	1.748024	-2.735841	2.883432
6	0.387737	-4.746728	-0.821804

6	-0.152378	-5.691196	-1.900592
1	0.499780	-5.284870	0.125032
1	1.390525	-4.402553	-1.105078
1	0.511578	-6.551846	-2.041868
1	-1.143881	-6.076313	-1.631335
1	-0.247158	-5.181307	-2.867322
1	0.113373	-3.003090	3.546682
15	-2.292812	-0.229081	0.335323
6	-2.442029	1.545385	-0.029889
6	-3.282003	-1.137399	-0.996485
6	-3.249166	-0.527766	1.926626
6	-3.672838	2.211288	-0.143040
6	-1.217697	2.221513	-0.300794
6	-2.727856	-0.778701	-2.385207
6	-4.809776	-0.974098	-0.962999
1	-3.050238	-2.192641	-0.803443
1	-4.261767	-0.135579	1.761824
6	-2.613634	0.258375	3.083033
6	-3.352605	-2.025397	2.256530
6	-3.775416	3.521841	-0.607168
1	-4.583961	1.687298	0.134990
6	-1.345156	3.520183	-0.868167
7	-0.016560	1.571359	-0.065486
1	-2.941055	0.267025	-2.632601
1	-3.195031	-1.410508	-3.151525
1	-1.642701	-0.917533	-2.425510
1	-5.107809	0.047009	-1.218342
1	-5.262060	-1.640214	-1.709160
1	-5.247576	-1.228273	0.008020
1	-2.573917	1.330486	2.867359
1	-3.198354	0.115848	4.000889
1	-1.590102	-0.082870	3.272495
1	-3.881654	-2.588928	1.480343
1	-3.900953	-2.166076	3.196526
1	-2.360675	-2.473874	2.378462
6	-5.102886	4.235989	-0.701904
6	-2.577516	4.139011	-1.008600
1	-0.459410	4.036317	-1.218264
6	1.173383	2.268689	0.092093
1	-5.255874	4.679910	-1.694138
1	-5.937587	3.551680	-0.513574
1	-5.180764	5.054027	0.027564
1	-2.613430	5.134259	-1.449326
6	1.278884	3.627520	0.495770
6	2.405957	1.579719	-0.089779
1	0.383568	4.172335	0.769889
6	2.504222	4.272259	0.575948
6	3.627851	2.265544	-0.038998
15	2.259634	-0.225030	-0.293494
1	2.524842	5.313888	0.893131
6	3.712466	3.623387	0.270304
1	4.548244	1.721381	-0.235483
6	2.867151	-0.566935	-2.041489
6	3.546671	-1.023390	0.846487
6	5.032369	4.357110	0.298169
6	2.069392	0.267501	-3.055614
1	3.913735	-0.235059	-2.068259
6	2.806047	-2.059559	-2.395402
6	4.994351	-1.105242	0.331800
1	3.171754	-2.050637	0.943296
6	3.507031	-0.366660	2.237777

1	5.124020	5.065866	-0.536563
1	5.155794	4.936829	1.221938
1	5.876575	3.662230	0.228393
1	2.438516	0.073083	-4.070871
1	2.162537	1.339295	-2.858137
1	1.005127	0.010622	-3.020450
1	3.234949	-2.229506	-3.391158
1	1.767110	-2.403746	-2.414331
1	3.356628	-2.688807	-1.686890
1	5.075892	-1.619835	-0.629770
1	5.449839	-0.115484	0.227354
1	5.602989	-1.664258	1.054399
1	3.957024	0.630388	2.212413
1	2.484356	-0.254962	2.608898
1	4.071821	-0.975384	2.955573

Structure 18 - NBE

B3LYP/GBS(1) = -2128.857986 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2129.349701 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2128.200618 a.u.
Enthalpy Correction = 0.797408
Gibbs Free Energy Correction = 0.678201

Atomic No	x-coord	y-coord	z-coord
8	-0.376428	-2.631650	2.424135
77	0.017537	-0.721049	0.102481
6	0.333827	-2.499438	1.232510
1	1.402424	-2.677823	1.379077
6	0.245759	-2.007384	3.535914
1	0.360407	-0.928205	3.372124
1	1.234437	-2.448210	3.735138
6	-0.266322	-2.905163	0.013568
1	-1.323559	-3.156766	0.103153
6	0.450381	-3.811870	-0.974196
6	-0.249845	-3.921537	-2.332590
1	0.506160	-4.822939	-0.536525
1	1.488242	-3.486924	-1.113185
1	0.287561	-4.599769	-3.006011
1	-1.268164	-4.313405	-2.214201
1	-0.330169	-2.945412	-2.821583
1	-0.398163	-2.182252	4.401428
15	-2.311412	-0.385342	0.240859
6	-2.407670	1.413880	-0.059751
6	-3.210796	-1.190623	-1.218341
6	-3.442032	-0.677656	1.716200
6	-3.610602	2.121724	-0.203358
6	-1.160401	2.070890	-0.236981
6	-2.563091	-0.740983	-2.538623
6	-4.735323	-1.008316	-1.280710
1	-3.001079	-2.259605	-1.085282
1	-4.402988	-0.223568	1.439236
6	-2.908508	0.058392	2.953775
6	-3.668441	-2.170549	2.005048

6	-3.652381	3.459157	-0.599710
1	-4.550876	1.612950	-0.006757
6	-1.214325	3.402736	-0.722164
7	0.026984	1.373301	-0.004507
1	-2.748409	0.322987	-2.723224
1	-2.987051	-1.308503	-3.376764
1	-1.480501	-0.900262	-2.523155
1	-5.005640	0.035853	-1.465200
1	-5.135979	-1.598870	-2.114751
1	-5.245063	-1.341437	-0.371630
1	-2.787290	1.129978	2.766798
1	-3.607497	-0.064193	3.790994
1	-1.939619	-0.346164	3.258294
1	-4.095062	-2.702846	1.147587
1	-4.371604	-2.280851	2.840727
1	-2.729869	-2.658135	2.281817
6	-4.954579	4.213334	-0.731191
6	-2.420673	4.066736	-0.892211
1	-0.294093	3.914084	-0.978821
6	1.223670	2.046132	0.268160
1	-5.030536	4.725868	-1.698660
1	-5.815325	3.541408	-0.644009
1	-5.060596	4.982679	0.045928
1	-2.405358	5.088948	-1.266945
6	1.304284	3.336426	0.845831
6	2.454128	1.378128	0.033556
1	0.395235	3.850443	1.134831
6	2.527988	3.951192	1.078794
6	3.672469	2.036003	0.241207
15	2.266514	-0.367507	-0.480901
1	2.536086	4.940514	1.533404
6	3.745020	3.333520	0.754176
1	4.600459	1.519928	0.012251
6	2.723741	-0.315490	-2.313265
6	3.656813	-1.361244	0.337063
6	5.067070	4.032343	0.969251
6	1.819603	0.669454	-3.070506
1	3.749354	0.077674	-2.334702
6	2.704679	-1.692041	-2.991275
6	5.053871	-1.305509	-0.306867
1	3.297084	-2.395206	0.237243
6	3.744361	-1.039912	1.839981
1	5.199440	4.876375	0.278684
1	5.151833	4.436817	1.985963
1	5.909188	3.349081	0.813994
1	2.128052	0.719417	-4.122600
1	1.876036	1.678083	-2.651726
1	0.773607	0.348062	-3.035764
1	3.081075	-1.604666	-4.018475
1	1.685359	-2.082940	-3.042757
1	3.323663	-2.434475	-2.476495
1	5.049356	-1.593764	-1.361341
1	5.505653	-0.311552	-0.231117
1	5.719587	-2.001729	0.219431
1	4.164206	-0.043500	2.007564
1	2.765334	-1.067686	2.325436
1	4.394279	-1.769914	2.338885

Structure 38 - NBE

B3LYP/GBS(1) = -2128.853780 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2129.347159 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2128.193143 a.u.
Enthalpy Correction = 0.797275
Gibbs Free Energy Correction = 0.675976

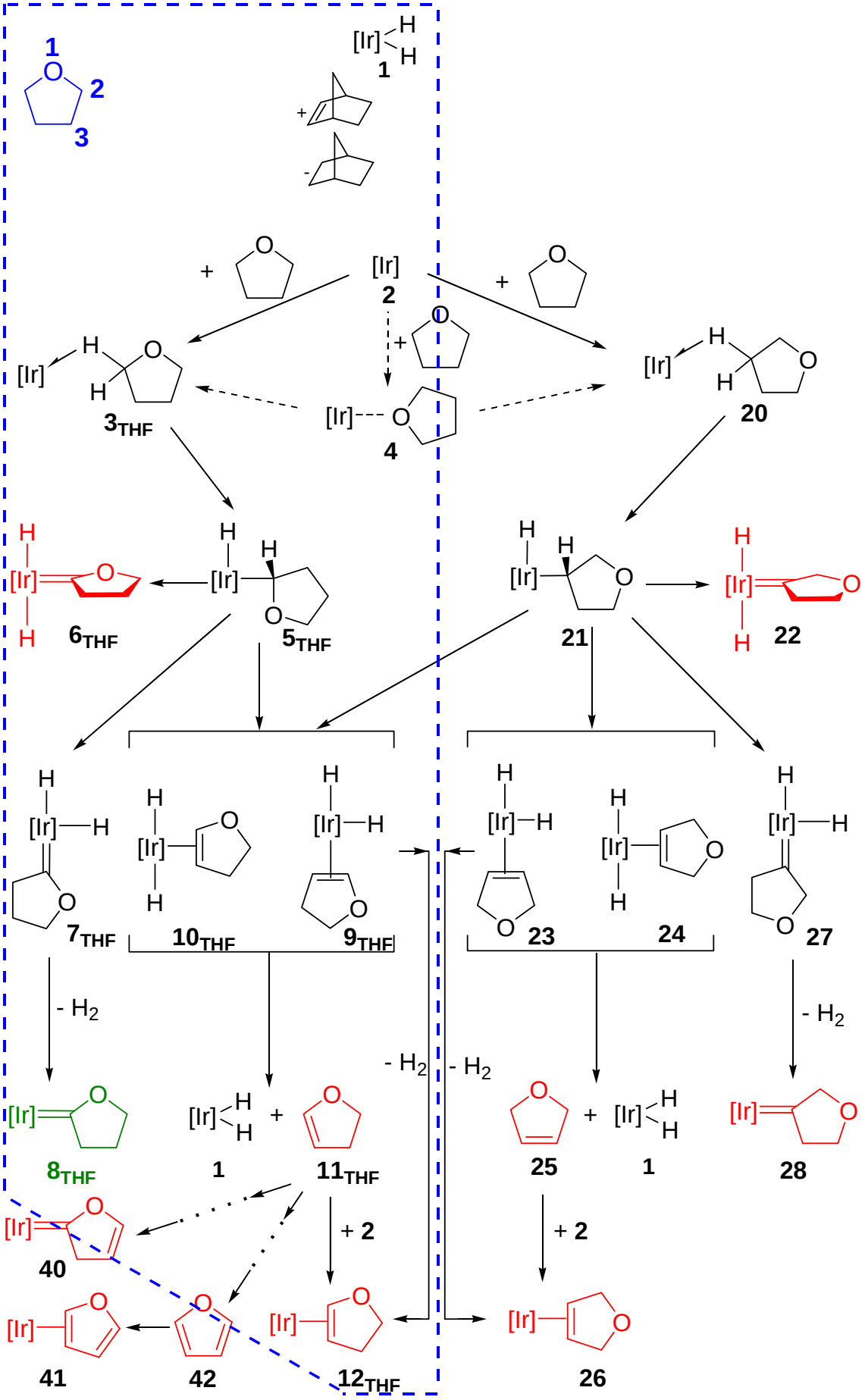
Atomic No	x-coord	y-coord	z-coord
77	0.002082	-0.540482	0.496027
6	0.097587	-2.703632	0.851650
1	-0.904342	-3.122205	0.750020
6	0.365562	-1.982527	2.044872
1	1.385559	-1.962338	2.424848
6	1.139865	-3.564315	0.173886
1	2.131752	-3.116301	0.283432
1	1.183910	-4.544725	0.674796
6	0.849188	-3.807254	-1.301604
1	-0.118311	-4.327138	-1.418938
1	0.770339	-2.848671	-1.838902
8	1.892636	-4.598693	-1.849346
6	1.684983	-4.911349	-3.208555
1	2.535892	-5.514100	-3.538084
1	0.758774	-5.491062	-3.355499
1	1.625147	-4.005484	-3.833810
1	-0.378719	-1.931093	2.836252
15	-2.333878	-0.459451	0.675225
6	-2.704703	0.986721	-0.376172
6	-3.287119	-1.920570	-0.050091
6	-3.190281	-0.079570	2.310519
6	-3.990261	1.377043	-0.777362
6	-1.561483	1.679483	-0.849506
6	-2.836313	-2.155223	-1.501269
6	-4.821778	-1.897609	0.045014
1	-2.933591	-2.765657	0.556357
1	-4.217862	0.202834	2.041843
6	-2.520982	1.128484	2.984776
6	-3.251816	-1.282625	3.264865
6	-4.205244	2.387206	-1.716762
1	-4.854068	0.876118	-0.349829
6	-1.781415	2.644044	-1.863265
7	-0.297104	1.340545	-0.352636
1	-3.182148	-1.344228	-2.151545
1	-3.257634	-3.094941	-1.880418
1	-1.746182	-2.204310	-1.577572
1	-5.254298	-1.158944	-0.635751
1	-5.216415	-2.878192	-0.251017
1	-5.188624	-1.690605	1.055029
1	-2.513076	2.004432	2.328680
1	-3.063455	1.394556	3.900998
1	-1.483483	0.901349	3.253034
1	-3.724946	-2.160809	2.813408
1	-3.832719	-1.017531	4.157224
1	-2.252610	-1.574787	3.602642
6	-5.595786	2.808021	-2.130875
6	-3.062931	2.981073	-2.277075
1	-0.931300	3.123977	-2.334091
6	0.730741	2.288791	-0.310371

1	-5.716277	2.793765	-3.221686
1	-6.356549	2.144771	-1.705145
1	-5.828068	3.828635	-1.797915
1	-3.179501	3.727810	-3.060763
6	0.526032	3.691299	-0.342744
6	2.069852	1.850019	-0.149353
1	-0.482889	4.085188	-0.358241
6	1.591348	4.581206	-0.336565
6	3.128216	2.768361	-0.190310
15	2.274465	0.057744	0.160661
1	1.378840	5.648833	-0.360125
6	2.924487	4.145301	-0.298950
1	4.149153	2.402840	-0.127484
6	3.400485	-0.429936	-1.282129
6	3.355870	-0.103817	1.704926
6	4.076563	5.120738	-0.356062
6	2.669202	-0.235191	-2.619775
1	4.203892	0.317149	-1.230743
6	4.045094	-1.822725	-1.201585
6	4.839607	0.287486	1.595117
1	3.313561	-1.180879	1.918716
6	2.693870	0.642515	2.877145
1	4.176744	5.575736	-1.351090
1	3.947290	5.943562	0.358472
1	5.027868	4.628666	-0.125972
1	3.358434	-0.428987	-3.451645
1	2.285316	0.783549	-2.728154
1	1.824479	-0.925786	-2.714185
1	4.859188	-1.883013	-1.935802
1	3.341494	-2.624314	-1.439491
1	4.479992	-2.036783	-0.219463
1	5.355800	-0.196773	0.761125
1	4.963102	1.369820	1.492851
1	5.357779	-0.008817	2.516318
1	2.746636	1.725848	2.724181
1	1.639726	0.371145	2.985837
1	3.215313	0.407603	3.813790

3. Tetrahydrofuran (THF)

3.1. Tetrahydrofuran (THF) relative energy diagrams.

Scheme S3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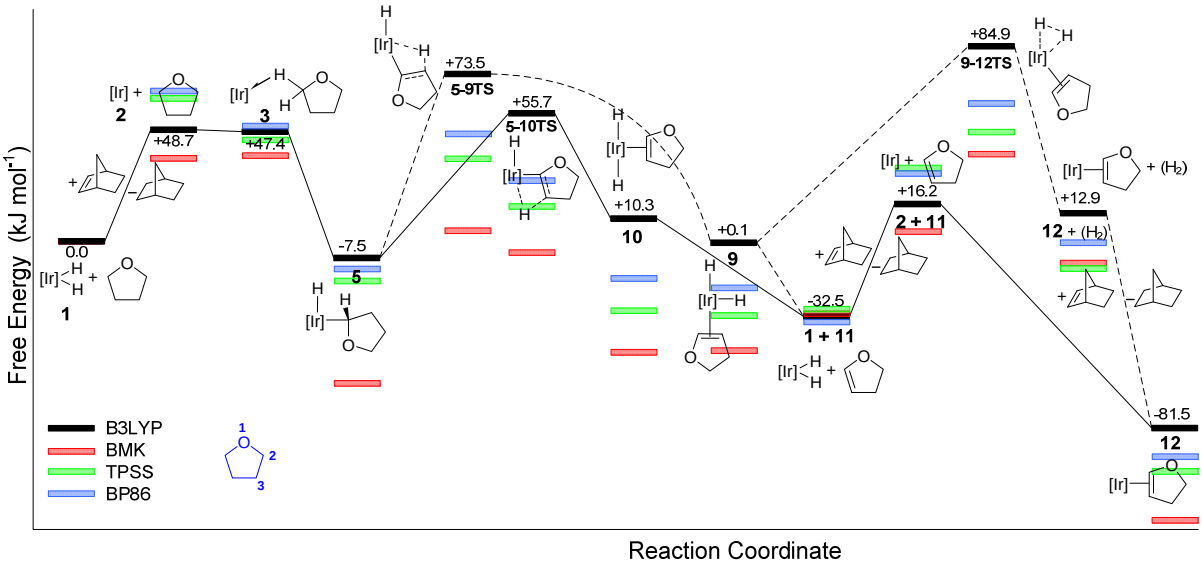


Figure S16. Relative energy surface for the formation of vinyl ether adduct $\mathbf{12}_{\mathbf{THF}}$. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

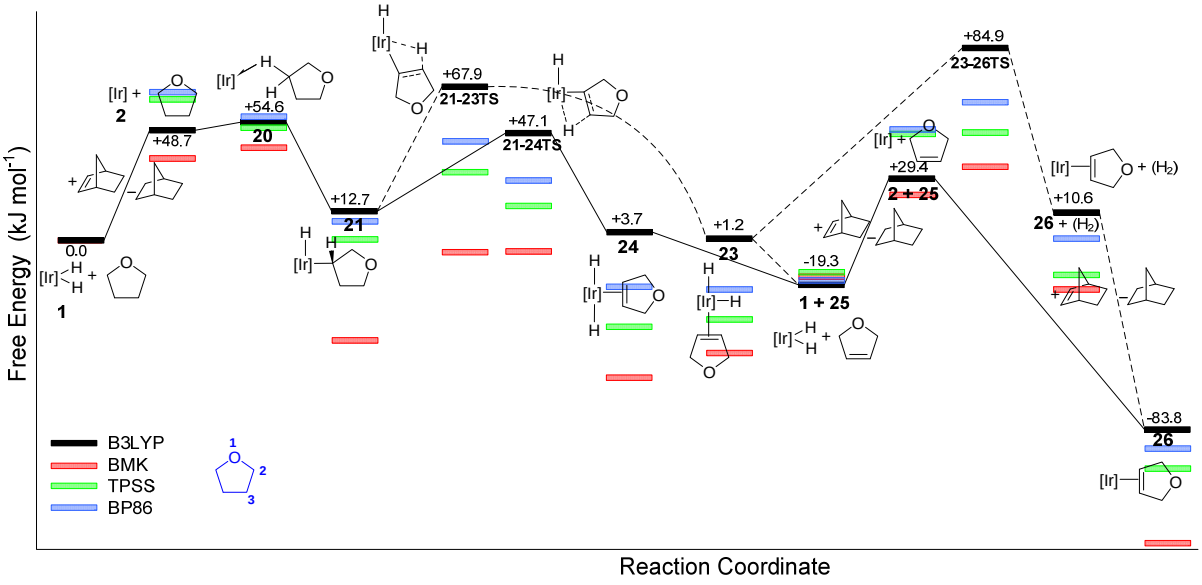


Figure S17. Relative energy surface for the formation of vinyl ether adduct $\mathbf{26}_{\mathbf{THF}}$. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

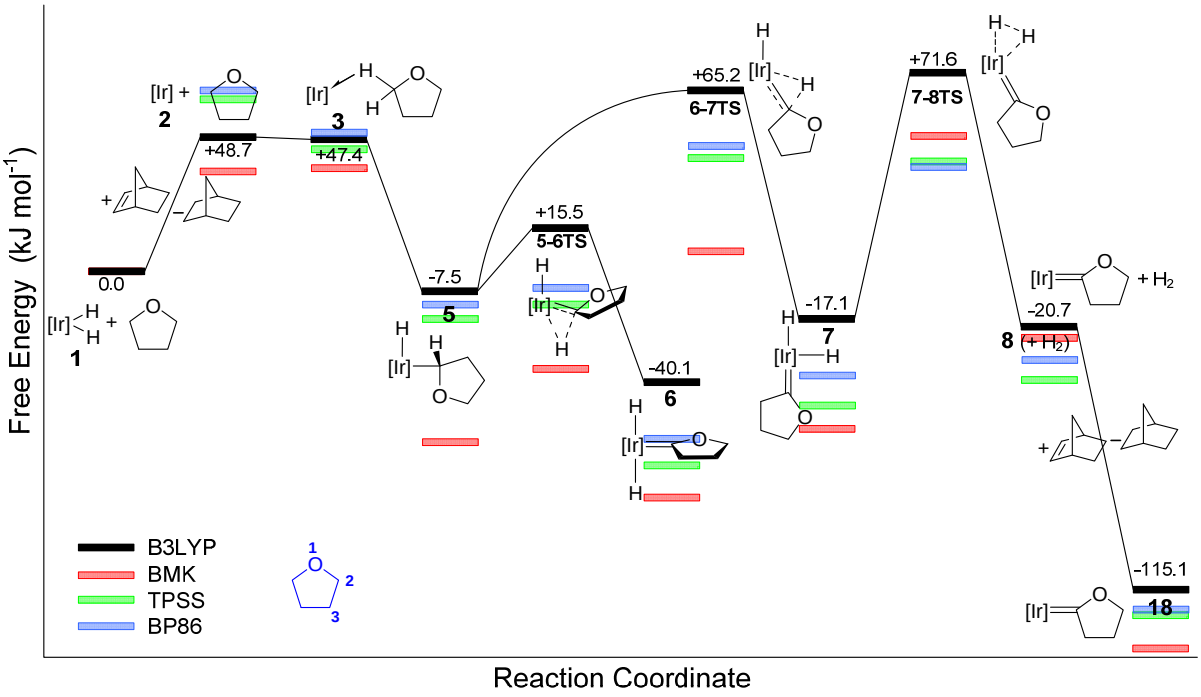


Figure S18. Relative energy surface for the formation of carbene $\mathbf{18}_{\mathbf{THF}}$. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

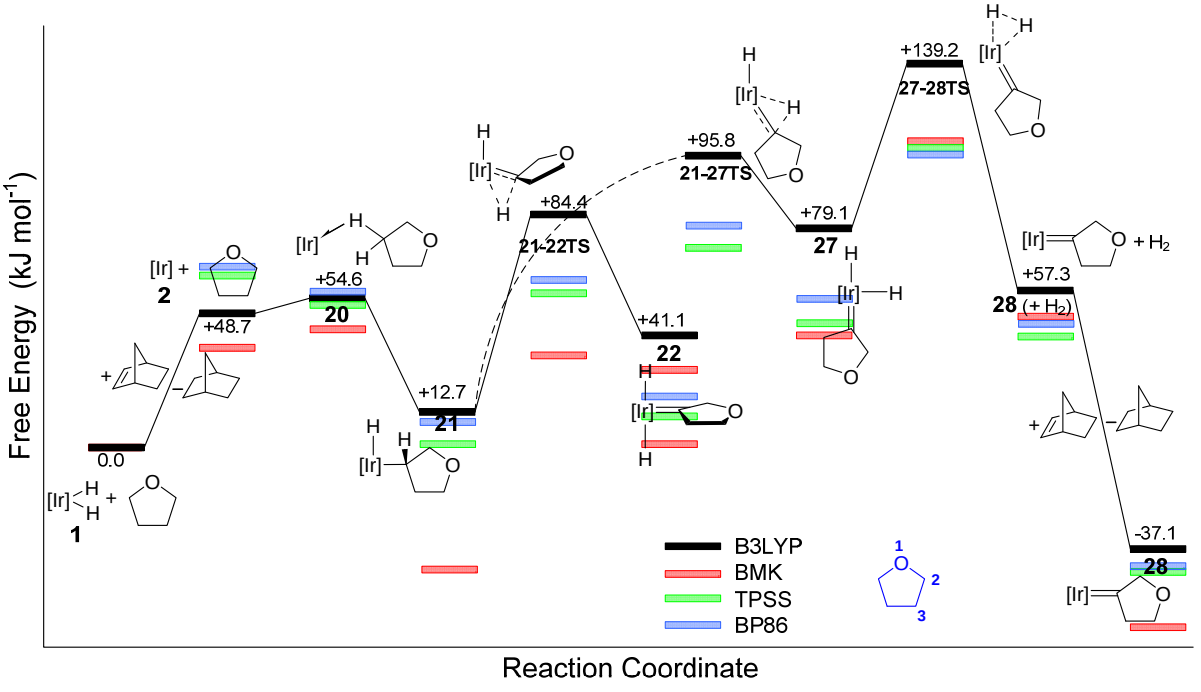


Figure S19. Relative energy surface for the formation of carbene $\mathbf{28}_{\mathbf{THF}}$. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

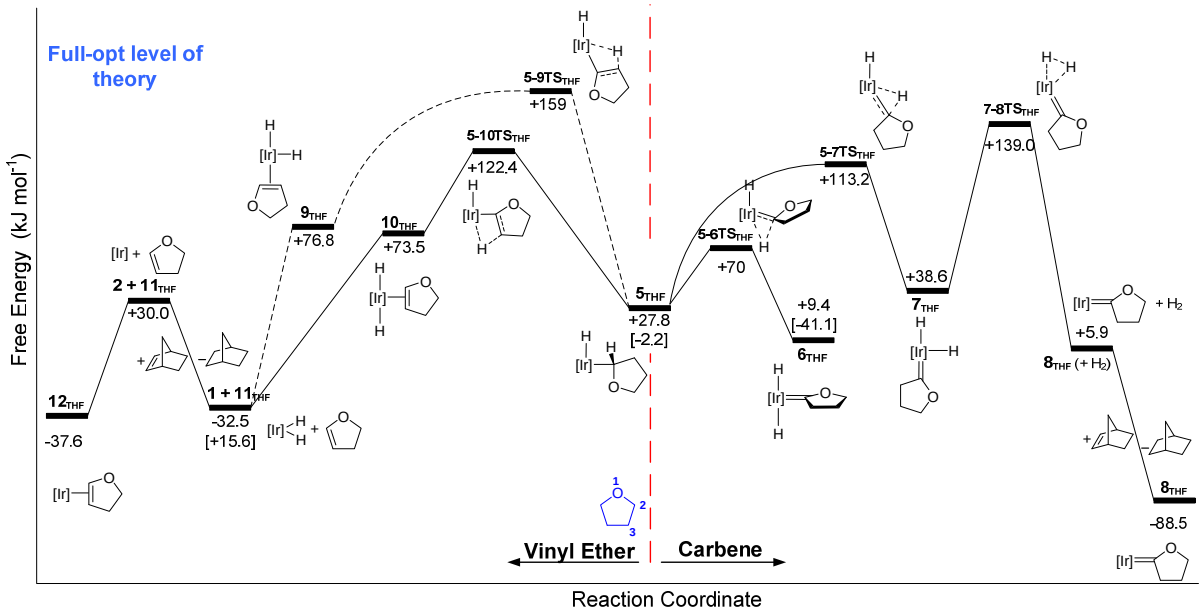


Figure S20. Relative energy surface for the formation of carbene and vinyl ether products. Values are B3LYP Gibbs corrected Full-opt energies. Those in square brackets are MP2 Gibbs corrected Full-opt energies. Drawn to scale with all values in kJ mol^{-1}.

3.2. Coordinates of THF structures at the Model-opt level of theory

Structure THF
B3LYP/GBS(1) = -232.445608 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -232.524512 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -232.368395 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -232.558083 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -232.516646 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -231.875834 a.u.
Enthalpy Correction = 0.123318
Gibbs Free Energy Correction = 0.08878

Atomic No	x-coord	y-coord	z-coord
6	1.165271	-0.430889	-0.131731
8	0.000141	-1.251095	-0.000333
6	-1.165047	-0.431201	0.132150
6	-0.733959	0.996683	-0.227051
6	0.733576	0.997011	0.226863
1	1.948583	-0.823526	0.527364
1	1.535628	-0.483256	-1.167510
1	-1.948840	-0.824209	-0.526134
1	-1.534449	-0.483395	1.168297
1	-0.797018	1.154809	-1.310496
1	-1.344272	1.761365	0.263604
1	1.343644	1.761699	-0.264083
1	0.796547	1.155654	1.310237

Structure 3 - THF

B3LYP/GBS(1) = -1389.123554 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.410590 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.209859 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.478837 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.5308222 a.u.
Enthalpy Correction = 0.368639
Gibbs Free Energy Correction = 0.293042

Atomic No	x-coord	y-coord	z-coord
7	2.033131	1.135217	-0.061498
6	3.228701	0.469273	-0.107453
6	3.315203	-0.888737	-0.097461
1	4.122797	1.094395	-0.155512
1	4.274809	-1.394748	-0.134148
6	2.011278	2.506142	-0.099248
6	0.858356	3.227565	-0.079078
1	2.985909	2.996312	-0.149046
1	0.872549	4.312574	-0.108405
15	1.730760	-1.722077	-0.020814
15	-0.628749	2.229004	0.003868
6	1.822820	-2.896026	1.415698
1	0.909202	-3.498534	1.474588
1	2.682577	-3.570253	1.324036
1	1.918953	-2.317870	2.338747
6	1.689066	-2.915686	-1.441959
1	2.558410	-3.583646	-1.426856
1	0.778813	-3.524469	-1.400307
1	1.687689	-2.349921	-2.377406
6	-1.613410	2.816431	1.458994
1	-1.857747	3.881985	1.374531
1	-2.540031	2.236736	1.520563
1	-1.032623	2.653096	2.370946
6	-1.723727	2.743678	-1.399081
1	-2.667302	2.191929	-1.338896
1	-1.935895	3.818807	-1.366885
1	-1.231140	2.501674	-2.344515
77	0.290869	0.100190	0.022639
6	-1.946567	-1.079777	0.459477
8	-3.115692	-0.277525	0.358568
6	-4.010867	-0.945212	-0.530828
6	-3.872352	-2.426484	-0.165353
6	-2.363320	-2.544297	0.146969
1	-1.248782	-0.781235	-0.432383
1	-1.513806	-0.938499	1.449468
1	-5.009093	-0.530776	-0.367444
1	-3.719047	-0.764644	-1.578850
1	-4.469469	-2.643248	0.726707
1	-4.196845	-3.097951	-0.966149
1	-2.164668	-3.209783	0.991949
1	-1.809837	-2.927983	-0.715832

Structure 4 – THF (Ether attached via the oxygen)
B3LYP/GBS(1) = -1389.139136 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.420975 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.223774 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.487922 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.537135 a.u.
Enthalpy Correction = 0.370010
Gibbs Free Energy Correction = 0.293711

Atomic No	x-coord	y-coord	z-coord
7	1.851276	1.323883	-0.017802
6	1.707077	2.683842	-0.030048
6	0.487263	3.289273	-0.025122
1	2.630080	3.267765	-0.043554
1	0.391139	4.370729	-0.032668
6	3.107376	0.780718	-0.022319
6	3.326905	-0.563815	-0.012620
1	3.938537	1.489448	-0.034392
1	4.332660	-0.972550	-0.016548
15	-0.894902	2.149995	0.005080
15	1.828364	-1.543617	0.004666
6	-2.000952	2.646135	-1.407783
1	-2.935025	2.072110	-1.384561
1	-2.248615	3.713632	-1.364516
1	-1.485857	2.438049	-2.349654
6	-1.954006	2.678260	1.442038
1	-2.192449	3.747358	1.387933
1	-2.893466	2.113276	1.458707
1	-1.411279	2.480521	2.370424
6	1.957445	-2.740785	-1.412422
1	2.878970	-3.332546	-1.354225
1	1.101503	-3.425735	-1.407997
1	1.951547	-2.180058	-2.351094
6	1.968452	-2.716807	1.439585
1	1.102995	-3.389152	1.461035
1	2.881458	-3.321176	1.376956
1	1.984679	-2.139234	2.367799
77	0.214974	0.113255	0.005399
6	-2.237231	-1.513446	-1.196659
8	-1.494324	-1.265312	0.023437
6	-2.384242	-1.353943	1.151728
6	-3.352109	-2.462435	0.748264
6	-3.556690	-2.185622	-0.756089
1	-2.398017	-0.562174	-1.712867
1	-1.603557	-2.146684	-1.821734
1	-1.767966	-1.565394	2.026411
1	-2.895267	-0.392209	1.297978
1	-2.885662	-3.441194	0.905118
1	-4.286638	-2.433745	1.316426
1	-3.764685	-3.096799	-1.324130
1	-4.400105	-1.503487	-0.906986

Structure 5 - THF
B3LYP/GBS(1) = -1389.140762 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.428977 a.u.

BMK/GBS(2)//B3LYP/GBS(1) = -1388.245629 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.499795 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.551540 a.u.
Enthalpy Correction = 0.364793
Gibbs Free Energy Correction = 0.290543

Atomic No	x-coord	y-coord	z-coord
7	1.394544	-1.883089	0.008805
6	2.745380	-1.735756	0.062706
6	3.350742	-0.510511	0.058037
1	3.347297	-2.648720	0.113753
1	4.432422	-0.421270	0.097558
6	0.792396	-3.103859	0.091959
6	-0.564397	-3.255174	0.117792
1	1.447681	-3.979299	0.141360
1	-1.012713	-4.242328	0.180412
15	2.261162	0.916384	-0.010784
15	-1.532312	-1.740525	0.046750
6	2.826541	1.944397	-1.447152
1	2.251476	2.875233	-1.494379
1	3.891578	2.188570	-1.360482
1	2.668462	1.387632	-2.375497
6	2.698738	2.006602	1.418719
1	3.765997	2.255467	1.408569
1	2.114599	2.931574	1.380652
1	2.463932	1.482322	2.348887
6	-2.700971	-1.878020	-1.378930
1	-3.369470	-2.738782	-1.263300
1	-3.286684	-0.955807	-1.427684
1	-2.133859	-1.993366	-2.307534
6	-2.675277	-1.701262	1.492436
1	-3.231887	-0.761214	1.454075
1	-3.368172	-2.550147	1.478234
1	-2.087516	-1.731963	2.413742
77	0.147902	-0.122851	-0.064735
6	-1.102437	1.504706	-0.345359
8	-2.503518	1.227801	-0.070096
6	-3.209054	2.454596	-0.220800
6	-2.251360	3.577713	0.255145
6	-0.890080	2.846801	0.381508
1	0.083342	-0.017285	1.481737
1	-1.034672	1.711343	-1.444349
1	-3.484020	2.607125	-1.278423
1	-4.132791	2.388538	0.364025
1	-2.213597	4.394907	-0.473369
1	-2.571648	4.006995	1.210252
1	-0.065074	3.421908	-0.055546
1	-0.650865	2.667994	1.435174

Structure 5-6TS - THF

B3LYP/GBS(1) = -1389.125714 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.418146 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.234010 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.495969 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.547381 a.u.
Enthalpy Correction = 0.360022
Gibbs Free Energy Correction = 0.288462
Imaginary Freq = -787.9 i

Atomic No	x-coord	y-coord	z-coord
7	0.874182	-2.051521	-0.507063
6	2.215186	-2.211520	-0.626508
6	3.096667	-1.197078	-0.390665
1	2.574893	-3.203598	-0.916614
1	4.167034	-1.344007	-0.501562
6	0.019772	-3.101269	-0.619461
6	-1.318804	-2.987807	-0.382210
1	0.453111	-4.064411	-0.906349
1	-1.982327	-3.840181	-0.494287
15	2.392846	0.371865	0.110417
15	-1.903290	-1.361651	0.096863
6	3.167053	1.622310	-1.025106
1	2.986730	2.644590	-0.676399
1	4.250474	1.462986	-1.075186
1	2.746799	1.507324	-2.028107
6	3.184224	0.838933	1.719452
1	4.277617	0.835866	1.640331
1	2.853901	1.837174	2.026927
1	2.873863	0.119981	2.481443
6	-3.255256	-0.925650	-1.088957
1	-4.029852	-1.701385	-1.095499
1	-3.699222	0.032145	-0.805719
1	-2.829873	-0.836905	-2.092223
6	-2.840862	-1.529499	1.680402
1	-3.245047	-0.552858	1.965964
1	-3.665040	-2.245637	1.582798
1	-2.155706	-1.868308	2.461243
77	0.084755	-0.129747	0.111927
6	-0.721564	1.638936	0.042011
8	-2.073936	1.832440	0.128764
6	-2.466590	3.204579	-0.123677
6	-1.214898	3.888973	-0.675626
6	-0.105522	3.031328	-0.050134
1	0.368740	-0.800734	1.561725
1	-0.380393	0.931601	-1.298975
1	-3.313209	3.188645	-0.816248
1	-2.796649	3.640173	0.827359
1	-1.183777	3.812251	-1.768228
1	-1.160937	4.947268	-0.404431
1	0.828125	3.040361	-0.609775
1	0.107056	3.362682	0.976407

Structure 5-7TS - THF
B3LYP/GBS(1) = -1389.106866 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.400966 a.u.

BMK/GBS(2)//B3LYP/GBS(1) = -1388.218634 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.477261 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.529471 a.u.
Enthalpy Correction = 0.362117
Gibbs Free Energy Correction = 0.290205
Imaginary Freq = -295.9 i

Atomic No	x-coord	y-coord	z-coord
7	0.804674	-2.042634	-0.427765
6	2.139358	-2.233703	-0.621886
6	3.059127	-1.248364	-0.437666
1	2.437889	-3.233233	-0.943660
1	4.115559	-1.425213	-0.614229
6	-0.075578	-3.076064	-0.578118
6	-1.410951	-2.943562	-0.364330
1	0.357312	-4.028359	-0.890176
1	-2.088450	-3.778424	-0.514531
15	2.401922	0.343094	0.048775
15	-1.960396	-1.292368	0.065956
6	3.120828	1.545212	-1.169433
1	2.910361	2.579021	-0.879808
1	4.207502	1.412842	-1.232589
1	2.681769	1.359430	-2.153250
6	3.266940	0.863053	1.603196
1	4.355094	0.857577	1.471583
1	2.952042	1.872530	1.890621
1	2.995817	0.171139	2.404479
6	-3.236642	-0.847865	-1.194768
1	-4.045234	-1.588272	-1.196753
1	-3.632859	0.145806	-0.979747
1	-2.762782	-0.828927	-2.179687
6	-2.975511	-1.393115	1.608128
1	-3.379619	-0.402136	1.840247
1	-3.807690	-2.096612	1.489497
1	-2.339689	-1.719106	2.435143
77	0.107008	-0.191877	0.192853
6	-0.674155	1.668730	-0.157588
8	-2.071253	1.881424	-0.299656
6	-2.395360	3.283004	-0.293943
6	-1.096579	4.027898	0.037689
6	-0.033618	3.024213	-0.442294
1	-2.775305	3.554909	-1.288753
1	-3.193623	3.460107	0.437111
1	-1.037791	5.005208	-0.452149
1	-1.006993	4.184545	1.119473
1	0.134528	3.136578	-1.521214
1	0.927546	3.149580	0.062013
1	-0.480660	1.450688	1.016955
1	0.422903	-0.995658	1.566472

Structure 5-9TS - THF
B3LYP/GBS(1) = -1389.101827 a.u.

B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.398144 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.219747 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.479180 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.529117 a.u.
Enthalpy Correction = 0.360279
Gibbs Free Energy Correction = 0.290552
Imaginary Freq = -648.4 i

Atomic No	x-coord	y-coord	z-coord
7	0.557606	-1.642694	-1.013946
6	-0.430565	-2.531659	-1.321776
6	-1.686560	-2.439129	-0.811512
1	-0.156091	-3.342144	-2.000896
1	-2.457841	-3.153922	-1.081625
6	1.838672	-1.863607	-1.413406
6	2.888805	-1.098202	-0.999752
1	1.995276	-2.708667	-2.088147
1	3.899885	-1.296554	-1.341330
15	-1.972017	-1.076604	0.318370
15	2.476298	0.197596	0.158814
6	-2.519813	-1.802538	1.930284
1	-2.748973	-1.000083	2.640052
1	-3.409808	-2.429697	1.801831
1	-1.702341	-2.401427	2.337695
6	-3.536496	-0.278678	-0.261486
1	-4.315479	-1.037712	-0.396504
1	-3.891112	0.456381	0.469518
1	-3.333646	0.227531	-1.206245
6	3.470350	-0.061359	1.696146
1	4.543734	-0.091982	1.475546
1	3.274465	0.748278	2.407583
1	3.161075	-1.004914	2.151265
6	3.239952	1.762060	-0.484172
1	3.100141	2.581911	0.229732
1	4.315259	1.624357	-0.644693
1	2.776723	2.039050	-1.435064
77	0.151634	-0.058240	0.292169
6	-0.317266	1.649943	-1.008751
8	-1.623104	1.840408	-1.552773
6	-2.218100	2.923080	-0.840394
6	-1.675781	2.820342	0.598534
6	-0.288008	2.199339	0.348306
1	0.456559	1.946166	-1.716107
1	-1.921907	3.884144	-1.293870
1	-3.306258	2.828102	-0.909209
1	-1.601065	3.794659	1.092189
1	-2.303263	2.175870	1.220574
1	0.570593	2.798042	0.645225
1	-0.179365	1.238210	1.383320
1	0.483891	-1.107963	1.532097

Structure 5-10TS - THF

B3LYP/GBS(1) = -1389.108768 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.404041 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.222956 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.486257 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.536094 a.u.
Enthalpy Correction = 0.35988
Gibbs Free Energy Correction = 0.289666
Imaginary Freq = -839.9 i

Atomic No	x-coord	y-coord	z-coord
7	0.854735	1.947531	-0.496408
6	-0.029247	2.979895	-0.556202
6	-1.358541	2.826716	-0.300640
1	0.379057	3.961668	-0.813008
1	-2.041563	3.668233	-0.369184
6	2.191209	2.152999	-0.604185
6	3.110776	1.167629	-0.386249
1	2.514839	3.164181	-0.867989
1	4.174642	1.357926	-0.490027
15	-1.896848	1.174704	0.148365
15	2.453309	-0.416512	0.119801
6	-3.338401	0.814581	-0.958209
1	-3.807852	-0.133594	-0.679350
1	-4.085892	1.611900	-0.872113
1	-3.000420	0.761561	-1.996711
6	-2.729287	1.248647	1.794295
1	-3.618088	1.889559	1.770697
1	-3.012361	0.231241	2.081127
1	-2.017984	1.634553	2.528101
6	3.200135	-1.691660	-1.001248
1	4.293289	-1.613889	-0.998168
1	2.925797	-2.702841	-0.679629
1	2.838364	-1.531279	-2.020840
6	3.236908	-0.864580	1.734692
1	2.897193	-1.855981	2.054616
1	4.330562	-0.870989	1.660132
1	2.927280	-0.132788	2.484520
77	0.141717	0.004225	0.073501
6	-0.581438	-1.901892	0.629048
8	-1.971993	-2.032280	0.919890
6	-2.558045	-2.758390	-0.164225
6	-1.753388	-2.367023	-1.421789
6	-0.391687	-2.009590	-0.809871
1	0.037720	-2.469849	1.322336
1	-2.478607	-3.841868	0.022986
1	-3.619929	-2.497779	-0.216551
1	-1.657200	-3.201944	-2.124429
1	-2.208107	-1.532950	-1.959125
1	0.477600	-2.531058	-1.196154
1	0.333043	0.582191	1.597969
1	-0.041689	-0.602907	-1.538075

Structure 6 - THF

B3LYP/GBS(1) = -1389.148703 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.439720 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.251653 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.518432 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.568744 a.u.
Enthalpy Correction = 0.361467
Gibbs Free Energy Correction = 0.288837

Atomic No	x-coord	y-coord	z-coord
7	-0.764226	-2.175654	-0.027093
6	-2.097560	-2.422541	-0.022274
6	-3.026849	-1.424563	-0.003266
1	-2.408634	-3.471523	-0.034363
1	-4.090166	-1.644941	-0.001829
6	0.151616	-3.179353	-0.042172
6	1.495976	-2.950223	-0.038276
1	-0.237262	-4.201966	-0.057767
1	2.205407	-3.772125	-0.050911
15	-2.391965	0.251548	0.007104
15	2.001551	-1.230060	-0.007949
6	-3.200285	1.108881	1.437688
1	-2.940989	2.173370	1.446525
1	-4.291471	1.015028	1.388123
1	-2.838988	0.652441	2.362488
6	-3.197615	1.108673	-1.426819
1	-4.288477	1.010134	-1.378611
1	-2.946153	2.175351	-1.441601
1	-2.832785	0.651347	-2.349665
6	3.139384	-1.007620	1.431565
1	4.010007	-1.669924	1.360132
1	3.478456	0.032557	1.464648
1	2.587205	-1.227422	2.348408
6	3.144131	-0.957053	-1.434794
1	3.482081	0.083990	-1.431016
1	4.015109	-1.620696	-1.382752
1	2.595668	-1.145670	-2.360755
77	-0.064628	-0.138427	0.008026
6	0.606534	1.657105	0.043390
8	1.922252	1.947207	0.039198
6	2.198765	3.371691	0.127446
6	0.897636	4.044111	-0.303658
6	-0.136565	2.987506	0.113571
1	2.466610	3.596670	1.166758
1	3.058331	3.574027	-0.515112
1	0.749934	5.016853	0.173513
1	0.883089	4.188402	-1.389375
1	-0.456551	3.130381	1.155125
1	-1.033643	2.977844	-0.506708
1	-0.107188	-0.308261	1.682935
1	-0.106466	-0.247044	-1.671857

Structure 7 - THF

B3LYP/GBS(1) = -1389.148703 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.439720 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.251653 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.518432 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.568744 a.u.
Enthalpy Correction = 0.361467
Gibbs Free Energy Correction = 0.288837

Atomic No	x-coord	y-coord	z-coord
7	-0.764226	-2.175654	-0.027093
6	-2.097560	-2.422541	-0.022274
6	-3.026849	-1.424563	-0.003266
1	-2.408634	-3.471523	-0.034363
1	-4.090166	-1.644941	-0.001829
6	0.151616	-3.179353	-0.042172
6	1.495976	-2.950223	-0.038276
1	-0.237262	-4.201966	-0.057767
1	2.205407	-3.772125	-0.050911
15	-2.391965	0.251548	0.007104
15	2.001551	-1.230060	-0.007949
6	-3.200285	1.108881	1.437688
1	-2.940989	2.173370	1.446525
1	-4.291471	1.015028	1.388123
1	-2.838988	0.652441	2.362488
6	-3.197615	1.108673	-1.426819
1	-4.288477	1.010134	-1.378611
1	-2.946153	2.175351	-1.441601
1	-2.832785	0.651347	-2.349665
6	3.139384	-1.007620	1.431565
1	4.010007	-1.669924	1.360132
1	3.478456	0.032557	1.464648
1	2.587205	-1.227422	2.348408
6	3.144131	-0.957053	-1.434794
1	3.482081	0.083990	-1.431016
1	4.015109	-1.620696	-1.382752
1	2.595668	-1.145670	-2.360755
77	-0.064628	-0.138427	0.008026
6	0.606534	1.657105	0.043390
8	1.922252	1.947207	0.039198
6	2.198765	3.371691	0.127446
6	0.897636	4.044111	-0.303658
6	-0.136565	2.987506	0.113571
1	2.466610	3.596670	1.166758
1	3.058331	3.574027	-0.515112
1	0.749934	5.016853	0.173513
1	0.883089	4.188402	-1.389375
1	-0.456551	3.130381	1.155125
1	-1.033643	2.977844	-0.506708
1	-0.107188	-0.308261	1.682935
1	-0.106466	-0.247044	-1.671857

Structure 7-8TS - THF

B3LYP/GBS(1) = -1389.100583 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.394530 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.198602 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.473695 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.527868 a.u.
Enthalpy Correction = 0.358324
Gibbs Free Energy Correction = 0.286192
Imaginary Freq = -776.4 i

Atomic No	x-coord	y-coord	z-coord
7	0.414298	-2.045973	-0.763806
6	1.686645	-2.413387	-1.052136
6	2.761445	-1.637771	-0.732787
1	1.825410	-3.374403	-1.557695
1	3.772173	-1.946457	-0.983900
6	-0.641156	-2.857172	-1.031705
6	-1.920028	-2.529399	-0.694669
1	-0.423518	-3.804123	-1.535894
1	-2.749870	-3.187997	-0.934494
15	2.417673	-0.079062	0.085495
15	-2.157477	-0.944889	0.114949
6	3.391008	1.164098	-0.895700
1	3.434552	2.134268	-0.391521
1	4.414998	0.797546	-1.033012
1	2.930603	1.292611	-1.878846
6	3.391264	-0.075752	1.664811
1	4.451402	-0.280697	1.475951
1	3.300694	0.895238	2.164305
1	2.989698	-0.847544	2.326457
6	-3.492529	-0.105060	-0.854257
1	-4.327633	-0.799385	-1.005013
1	-3.846550	0.784249	-0.328270
1	-3.096614	0.198930	-1.825991
6	-3.045259	-1.271853	1.707967
1	-3.284060	-0.322421	2.199343
1	-3.974221	-1.828245	1.537324
1	-2.393727	-1.853938	2.364937
77	0.053274	-0.152285	0.283323
6	-0.361774	1.677072	-0.160275
8	-1.643345	2.144837	-0.268472
6	-1.711086	3.549818	-0.597410
6	-0.365467	4.113238	-0.152760
6	0.545175	2.893978	-0.365711
1	-1.865204	3.649569	-1.680615
1	-2.577880	3.967404	-0.078562
1	-0.063351	4.994513	-0.726246
1	-0.399949	4.388153	0.907503
1	0.934560	2.875232	-1.392672
1	1.401252	2.872689	0.309642
1	0.073778	-0.214716	1.971985
1	0.285654	-1.188980	1.754951

Structure 8 - THF

B3LYP/GBS(1) = -1387.954855 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1388.234907 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1387.043396 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1388.309199 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1388.362101 a.u.
Enthalpy Correction = 0.345135
Gibbs Free Energy Correction = 0.272329

Atomic No	x-coord	y-coord	z-coord
7	0.785677	-2.138681	0.015795
6	2.131716	-2.383194	0.002934
6	3.053376	-1.381778	-0.012775
1	2.446260	-3.431333	0.005179
1	4.118276	-1.594334	-0.020999
6	-0.116650	-3.170794	0.027168
6	-1.462582	-2.968121	0.030312
1	0.294546	-4.184855	0.033677
1	-2.156481	-3.803298	0.039400
15	2.379375	0.286990	-0.007997
15	-1.975745	-1.242215	0.010954
6	3.181669	1.158722	-1.436705
1	2.903722	2.218176	-1.440693
1	4.273996	1.080533	-1.386234
1	2.832601	0.704084	-2.367738
6	3.191512	1.136876	1.429879
1	4.282898	1.050696	1.372116
1	2.925207	2.199509	1.454294
1	2.844069	0.670804	2.355822
6	-3.121614	-1.039138	-1.427773
1	-3.982098	-1.714367	-1.354507
1	-3.472118	-0.003065	-1.457709
1	-2.574397	-1.251864	-2.350071
6	-3.121650	-1.002407	1.443908
1	-3.467991	0.035584	1.449966
1	-3.984952	-1.675496	1.385866
1	-2.575765	-1.195602	2.371268
77	0.073755	-0.143939	-0.001627
6	-0.617249	1.628688	-0.039412
8	-1.957879	1.899799	-0.055301
6	-2.255607	3.312750	-0.157538
6	-0.981062	4.013758	0.307460
6	0.085324	2.984463	-0.096699
1	-2.496085	3.539061	-1.204592
1	-3.137582	3.508872	0.457468
1	-0.847521	4.996030	-0.155124
1	-0.993904	4.146307	1.395112
1	0.420253	3.147403	-1.132214
1	0.973679	3.002275	0.537899

Structure 9 - THF

B3LYP/GBS(1) = -1389.133585 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.425967 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.239696 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.505277 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.554579 a.u.
Enthalpy Correction = 0.362861
Gibbs Free Energy Correction = 0.290403

Atomic No	x-coord	y-coord	z-coord
7	-0.389781	-1.231066	1.418893
6	0.656812	-1.995884	1.835469
6	1.842186	-2.045425	1.164633
1	0.505956	-2.593582	2.740152
1	2.666833	-2.646960	1.536731
6	-1.632064	-1.366269	1.946756
6	-2.740172	-0.793359	1.385732
1	-1.724694	-1.973483	2.853303
1	-3.718215	-0.908312	1.844553
15	1.965040	-1.073957	-0.345044
15	-2.491260	0.077694	-0.164019
6	2.337242	-2.245775	-1.728227
1	2.484837	-1.681985	-2.655800
1	3.236776	-2.836231	-1.519352
1	1.484580	-2.915197	-1.862505
6	3.591089	-0.196586	-0.205835
1	4.401846	-0.928440	-0.112585
1	3.777469	0.420306	-1.091336
1	3.575425	0.432675	0.685253
6	-3.549414	-0.733141	-1.445722
1	-4.599596	-0.765184	-1.133546
1	-3.469946	-0.184135	-2.390038
1	-3.186089	-1.751247	-1.604555
6	-3.369477	1.703357	0.019186
1	-3.330686	2.269257	-0.918396
1	-4.420067	1.538566	0.284240
1	-2.903261	2.296490	0.811113
77	-0.167621	-0.097564	-0.427569
6	0.435070	1.709193	1.148600
8	1.750896	1.906887	1.496620
6	2.293321	2.885478	0.570766
6	1.349963	2.901547	-0.649478
6	0.101873	2.233473	-0.080635
1	-0.199242	1.389169	1.963820
1	2.308856	3.853331	1.088801
1	3.319603	2.597376	0.338520
1	1.144306	3.925080	-0.982066
1	1.751995	2.346453	-1.501398
1	-0.885168	2.563276	-0.362465
1	-0.066786	0.491901	-1.933957
1	-0.531853	-1.460014	-1.192409

Structure 10 - THF

B3LYP/GBS(1) = -1389.128835 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.423259 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.241298 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.505726 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.554310 a.u.
Enthalpy Correction = 0.362337
Gibbs Free Energy Correction = 0.291572

Atomic No	x-coord	y-coord	z-coord
7	0.787493	2.018444	-0.034865
6	-0.133340	3.022499	-0.039124
6	-1.471191	2.788790	-0.024988
1	0.260451	4.041650	-0.052494
1	-2.186829	3.605109	-0.029614
6	2.119004	2.288611	-0.022206
6	3.074893	1.318021	0.001809
1	2.398440	3.345073	-0.031398
1	4.131505	1.565904	0.007212
15	-1.964981	1.064240	0.009115
15	2.460063	-0.358946	0.016588
6	-3.182147	0.902120	-1.380045
1	-3.676750	-0.073931	-1.372298
1	-3.950968	1.679793	-1.303405
1	-2.646490	1.020214	-2.325535
6	-3.028988	0.852719	1.506634
1	-3.960422	1.424426	1.424409
1	-3.251774	-0.205754	1.663136
1	-2.458632	1.206313	2.369140
6	3.267651	-1.254920	-1.388061
1	4.359276	-1.180038	-1.324498
1	2.992530	-2.315805	-1.379905
1	2.926702	-0.810367	-2.326158
6	3.209822	-1.220045	1.473964
1	2.910874	-2.274611	1.489015
1	4.304292	-1.169604	1.443859
1	2.849160	-0.739241	2.386564
77	0.142588	0.010612	-0.022422
6	-0.434090	-2.009235	0.775305
8	-1.735667	-2.233179	1.188328
6	-2.556887	-2.501305	0.030562
6	-1.637955	-2.445942	-1.215179
6	-0.285362	-2.063800	-0.626453
1	0.292903	-2.295793	1.522636
1	-3.018605	-3.484640	0.174604
1	-3.360048	-1.758761	-0.001685
1	-1.565647	-3.431077	-1.693561
1	-1.994821	-1.741226	-1.969640
1	0.601492	-2.469174	-1.097599
1	0.172159	0.198260	1.647242
1	0.190112	0.137985	-1.694968

Structure 11 - THF
B3LYP/GBS(1) = -231.217727 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -231.296731 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -231.145031 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -231.332681 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -231.292380 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -230.663175 a.u.
Enthalpy Correction = 0.098790
Gibbs Free Energy Correction = 0.065467

Atomic No	x-coord	y-coord	z-coord
6	1.202108	-0.059670	0.006141
8	0.403902	-1.168508	-0.048354
6	-0.967297	-0.698885	0.049872
6	-0.926437	0.849866	-0.043114
6	0.563659	1.111254	0.031289
1	-1.537009	-1.172022	-0.754472
1	-1.364696	-1.043625	1.011309
1	-1.488650	1.318063	0.774492
1	-1.362901	1.219551	-0.981875
1	1.026274	2.088642	0.058485
1	2.263557	-0.277932	0.013763

Structure 12 - THF
B3LYP/GBS(1) = -1387.939920 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1388.223750 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1387.039464 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1388.300787 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1388.352000 a.u.
Enthalpy Correction = 0.345026
Gibbs Free Energy Correction = 0.273984

Atomic No	x-coord	y-coord	z-coord
7	0.741404	2.004488	-0.008820
6	-0.192617	3.011112	-0.023656
6	-1.525764	2.764303	-0.031950
1	0.192209	4.034348	-0.025705
1	-2.251870	3.571418	-0.039779
6	2.075407	2.313868	0.021360
6	3.054061	1.368903	0.042941
1	2.328443	3.377547	0.027458
1	4.104716	1.640255	0.063672
15	-1.980420	1.021943	-0.002771
15	2.454544	-0.319477	0.018028
6	-3.223166	0.857392	-1.372082
1	-3.692065	-0.131212	-1.364040
1	-4.007152	1.617105	-1.273135
1	-2.713913	0.995502	-2.330025

6	-3.022003	0.818231	1.515479
1	-3.938933	1.415437	1.453603
1	-3.268641	-0.234961	1.669063
1	-2.432691	1.153813	2.373147
6	3.313282	-1.169356	-1.388849
1	4.402137	-1.092945	-1.290464
1	3.038488	-2.229730	-1.418710
1	3.004470	-0.702880	-2.328205
6	3.205233	-1.185222	1.475364
1	2.920399	-2.243657	1.475468
1	4.298824	-1.117018	1.456642
1	2.833874	-0.723261	2.394131
77	0.139852	0.002396	-0.047110
6	-0.358895	-1.935197	0.772387
8	-1.653263	-2.195508	1.219906
6	-2.486153	-2.517713	0.087513
6	-1.591966	-2.487970	-1.178338
6	-0.238667	-2.045965	-0.634986
1	0.375872	-2.208001	1.525371
1	-2.929779	-3.503375	0.271521
1	-3.305505	-1.792725	0.039056
1	-1.511158	-3.487372	-1.626253
1	-1.989049	-1.820442	-1.950116
1	0.644635	-2.461037	-1.112673

Structure 20 - THF

B3LYP/GBS(1) = -1389.119591 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.407561 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.208124 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.475481 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.52727 a.u.
Enthalpy Correction = 0.368737
Gibbs Free Energy Correction = 0.29278

Atomic No	x-coord	y-coord	z-coord
7	-2.340834	0.151822	-0.035262
6	-3.111751	-0.980713	-0.019370
6	-2.581408	-2.231807	0.016166
1	-4.191793	-0.822278	-0.035225
1	-3.212032	-3.115079	0.025771
6	-2.946739	1.381169	-0.052425
6	-2.247304	2.546801	-0.043307
1	-4.038255	1.374217	-0.071681
1	-2.749125	3.509069	-0.055569
15	-0.790832	-2.264860	0.029580
15	-0.470427	2.332074	0.001916
6	-0.282973	-3.365763	-1.376799
1	0.803154	-3.508382	-1.378833
1	-0.764488	-4.347735	-1.299984
1	-0.576543	-2.897302	-2.320025
6	-0.282246	-3.300006	1.483204
1	-0.746156	-4.292597	1.443747

1	0.806497	-3.421281	1.500108
1	-0.591458	-2.796063	2.402751
6	0.217680	3.322725	-1.409929
1	-0.107661	4.368133	-1.353802
1	1.312874	3.295715	-1.396382
1	-0.130531	2.890131	-2.351750
6	0.137561	3.321428	1.450148
1	1.232043	3.313740	1.490181
1	-0.201958	4.361693	1.383254
1	-0.248385	2.877227	2.371430
77	-0.318189	0.011397	0.000269
6	3.218628	1.024337	0.044762
8	4.482096	0.446183	0.360649
6	4.519076	-0.844961	-0.236151
6	3.111936	-1.413150	-0.019205
6	2.235444	-0.153385	-0.198388
1	2.929572	1.661477	0.885650
1	3.297879	1.652978	-0.856106
1	4.750994	-0.773634	-1.312999
1	5.313308	-1.415512	0.253331
1	2.857308	-2.208868	-0.725511
1	3.023113	-1.811557	0.997416
1	1.802332	-0.105236	-1.202662
1	1.450425	-0.146932	0.643119

Structure 21 - THF

B3LYP/GBS(1) = -1389.132176 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.421294 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.238887 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.492496 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.543852 a.u.
Enthalpy Correction = 0.365132
Gibbs Free Energy Correction = 0.290557

Atomic No	x-coord	y-coord	z-coord
7	-1.497656	1.750963	-0.304844
6	-2.839003	1.520315	-0.345376
6	-3.378396	0.276079	-0.179130
1	-3.488213	2.384537	-0.516828
1	-4.452231	0.120941	-0.220483
6	-0.980615	3.008425	-0.405251
6	0.354461	3.260195	-0.289707
1	-1.686416	3.825722	-0.582592
1	0.743337	4.270688	-0.374542
15	-2.208536	-1.053928	0.102921
15	1.411658	1.839624	0.027358
6	-2.547687	-2.361340	-1.165518
1	-1.886187	-3.219231	-1.005262
1	-3.588594	-2.700168	-1.111407
1	-2.361543	-1.955191	-2.163998
6	-2.684246	-1.916332	1.666875
1	-3.715754	-2.282872	1.618231

1	-2.011849	-2.762412	1.843794
1	-2.591912	-1.216024	2.501097
6	2.735842	1.883175	-1.269428
1	3.243750	2.854482	-1.273807
1	3.474416	1.096576	-1.084064
1	2.285913	1.718462	-2.252969
6	2.370045	2.235735	1.559473
1	3.100943	1.448082	1.765787
1	2.894143	3.192028	1.450608
1	1.677774	2.303243	2.402879
77	-0.167897	0.090099	0.051350
6	2.412195	-1.544892	0.916260
8	3.181403	-2.672124	0.466578
6	2.678736	-3.099100	-0.802321
6	1.523179	-2.144090	-1.172843
6	1.060710	-1.617110	0.208176
1	2.339531	-1.600909	2.008585
1	2.953705	-0.618683	0.659024
1	3.491968	-3.087448	-1.541890
1	2.322769	-4.136208	-0.711662
1	1.901189	-1.323166	-1.800493
1	0.734720	-2.653904	-1.738219
1	-0.211687	0.172849	1.600895
1	0.512478	-2.440536	0.693251

Structure 21-22TS - THF

B3LYP/GBS(1) = -1389.097232 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.391691 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.206896 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.469943 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.521225 a.u.
Enthalpy Correction = 0.359832
Gibbs Free Energy Correction = 0.288265
Imaginary Freq = -815.9 i

Atomic No	x-coord	y-coord	z-coord
7	0.258101	-2.200126	-0.540715
6	1.505657	-2.718581	-0.662361
6	2.629302	-1.993217	-0.400843
1	1.580373	-3.764028	-0.976342
1	3.618614	-2.424936	-0.519746
6	-0.843993	-2.979849	-0.674127
6	-2.101481	-2.519233	-0.423269
1	-0.684444	-4.015616	-0.988517
1	-2.971516	-3.156294	-0.550957
15	2.384059	-0.302305	0.134640
15	-2.238342	-0.816812	0.113442
6	3.520538	0.691428	-0.947321
1	3.665401	1.704364	-0.558888
1	4.499091	0.200142	-0.997985
1	3.103557	0.749111	-1.956649
6	3.215055	-0.109643	1.777585

1	4.273285	-0.389836	1.722303
1	3.139111	0.928904	2.117834
1	2.706749	-0.750666	2.501623
6	-3.549016	-0.086807	-0.979380
1	-4.416219	-0.756698	-1.012692
1	-3.880029	0.889299	-0.612485
1	-3.153631	0.026310	-1.992621
6	-3.109282	-0.815306	1.747237
1	-3.284483	0.213094	2.082209
1	-4.072213	-1.335005	1.681790
1	-2.474590	-1.317187	2.481217
77	0.026310	-0.134311	0.097501
6	-0.197022	1.781807	0.015333
6	0.076219	4.093785	-0.618241
6	0.848588	2.886576	-0.076037
1	0.101939	-0.902788	1.540003
1	-0.056424	0.808461	-1.401657
1	0.031651	4.068560	-1.720646
1	0.475371	5.063408	-0.307419
1	1.717299	2.608102	-0.670658
1	1.188203	3.096524	0.948798
8	-1.222002	3.952984	-0.052573
6	-1.516137	2.557762	-0.044486
1	-2.076692	2.275132	-0.946725
1	-2.143268	2.355021	0.830443

Structure 21-23TS - THF

B3LYP/GBS(1) = -1389.106042 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.401335 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.225307 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.482504 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.531253 a.u.
Enthalpy Correction = 0.361184
Gibbs Free Energy Correction = 0.291612
Imaginary Freq = -346.0 i

Atomic No	x-coord	y-coord	z-coord
7	0.494924	-1.652433	-1.001666
6	-0.516089	-2.531810	-1.265964
6	-1.764851	-2.391922	-0.750969
1	-0.263262	-3.374985	-1.912912
1	-2.552453	-3.100409	-0.989486
6	1.770477	-1.936998	-1.380289
6	2.848738	-1.210902	-0.968949
1	1.896846	-2.803056	-2.034338
1	3.853701	-1.459665	-1.295247
15	-2.021550	-0.977496	0.324493
15	2.481121	0.107171	0.179529
6	-2.522638	-1.627187	1.985619
1	-2.731043	-0.790318	2.661362
1	-3.417935	-2.255405	1.911539
1	-1.695325	-2.207779	2.398488

6	-3.641902	-0.270664	-0.232172
1	-4.403935	-1.057855	-0.181913
1	-3.942034	0.568196	0.399018
1	-3.567858	0.088585	-1.259714
6	3.407874	-0.217943	1.747016
1	4.484048	-0.311867	1.560360
1	3.238429	0.598672	2.457348
1	3.028985	-1.143452	2.186147
6	3.368175	1.618588	-0.429581
1	3.243987	2.449876	0.273631
1	4.439261	1.411824	-0.533970
1	2.973482	1.918302	-1.403618
77	0.142721	-0.024490	0.258393
6	-0.126876	1.738078	-1.049828
6	-1.538793	2.920425	0.476908
6	-0.164775	2.263721	0.326360
1	0.740195	1.978578	-1.659472
1	-1.406695	4.011143	0.357518
1	-2.046705	2.735298	1.428511
1	0.678186	2.850105	0.692188
1	-0.145385	1.327285	1.314866
1	0.393594	-1.064712	1.518310
8	-2.339571	2.387548	-0.563337
6	-1.470309	2.101961	-1.667661
1	-1.382696	2.997078	-2.312189
1	-1.940550	1.309733	-2.257563

Structure 21-24TS - THF

B3LYP/GBS(1) = -1389.114959 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.409093 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.230726 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.491401 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.540267 a.u.
Enthalpy Correction = 0.360641
Gibbs Free Energy Correction = 0.291434
Imaginary Freq = -823.4 i

Atomic No	x-coord	y-coord	z-coord
7	-0.718424	2.002159	-0.384634
6	-2.036892	2.299683	-0.493896
6	-3.024439	1.368563	-0.343122
1	-2.288351	3.343105	-0.704153
1	-4.071860	1.635207	-0.443799
6	0.226464	2.982844	-0.391538
6	1.542311	2.729823	-0.163148
1	-0.124383	4.000297	-0.584901
1	2.280170	3.526269	-0.193475
15	-2.472575	-0.274981	0.082991
15	1.991938	1.015713	0.133858
6	-3.264033	-1.455530	-1.107879
1	-3.019067	-2.491417	-0.846338
1	-4.354335	-1.345418	-1.096486

1	-2.899037	-1.247419	-2.117567
6	-3.296971	-0.766047	1.664684
1	-4.388538	-0.717416	1.577541
1	-3.009011	-1.787487	1.937022
1	-2.963986	-0.088672	2.454530
6	3.324740	0.672900	-1.105649
1	4.110824	1.433182	-1.028603
1	3.752484	-0.316495	-0.927801
1	2.897926	0.713769	-2.111849
6	2.959825	0.984566	1.709550
1	3.370992	-0.016280	1.875349
1	3.786794	1.702924	1.672198
1	2.295169	1.239379	2.538467
77	-0.143483	-0.006754	0.080439
6	1.648339	-2.503664	0.951985
8	2.491511	-2.231699	-0.174864
6	1.690606	-2.363550	-1.344420
6	0.273673	-1.989066	-0.928503
6	0.255401	-2.056338	0.532150
1	2.064808	-1.975959	1.813710
1	2.132287	-1.746941	-2.130393
1	1.678156	-3.413965	-1.687442
1	-0.532798	-2.426878	-1.510642
1	-0.567153	-2.565491	1.030735
1	1.656390	-3.586924	1.172446
1	0.035625	-0.551385	-1.556009
1	-0.282653	0.506434	1.630979

Structure 21-27TS - THF

B3LYP/GBS(1) = -1389.095933 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.391257 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.212955 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.467099 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.518312 a.u.
Enthalpy Correction = 0.362896
Gibbs Free Energy Correction = 0.292151
Imaginary Freq = -35.8 I (note, a very flat surface observed. The presence of an agostic C-H-Ir interactions flattening the transition to the point where an intermediate is almost observed)

Atomic No	x-coord	y-coord	z-coord
7	0.098296	-2.108254	-0.624435
6	1.306574	-2.701852	-0.850147
6	2.489162	-2.096247	-0.569778
1	1.270848	-3.703565	-1.281576
1	3.436160	-2.584408	-0.777021
6	-1.056995	-2.808791	-0.825809
6	-2.283083	-2.310677	-0.523850
1	-0.939964	-3.804792	-1.256060
1	-3.185489	-2.883892	-0.711863
15	2.365517	-0.449955	0.117149
15	-2.302899	-0.651562	0.147811
6	3.530425	0.571210	-0.902152

1	3.767750	1.519244	-0.411397
1	4.462294	0.015982	-1.059769
1	3.070829	0.781085	-1.871250
6	3.227083	-0.451508	1.756560
1	4.271492	-0.767327	1.652976
1	3.203076	0.551836	2.195856
1	2.705137	-1.138711	2.426894
6	-3.599199	0.225703	-0.847319
1	-4.504335	-0.391354	-0.891691
1	-3.854653	1.192610	-0.405173
1	-3.232089	0.387345	-1.864074
6	-3.121115	-0.718370	1.807623
1	-3.204747	0.289982	2.227292
1	-4.123754	-1.154246	1.732909
1	-2.508726	-1.326844	2.477182
77	0.017010	-0.204635	0.167297
6	-0.052103	1.822634	-0.255914
6	0.371919	4.150526	0.087382
6	1.063779	2.869552	-0.388100
1	0.814645	5.076734	-0.295348
1	0.365243	4.201167	1.191394
1	1.354683	2.985679	-1.440919
1	1.960359	2.630281	0.187872
1	-0.059393	1.587316	0.912771
1	0.048996	-1.133849	1.501612
8	-0.950421	4.056204	-0.428617
6	-1.312598	2.665711	-0.496761
1	-1.740973	2.501897	-1.493278
1	-2.094227	2.448284	0.245973

Structure 22 - THF

B3LYP/GBS(1) = -1389.113758 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.407817 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.218477 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.486042 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.537179 a.u.
Enthalpy Correction = 0.360673
Gibbs Free Energy Correction = 0.287890

Atomic No	x-coord	y-coord	z-coord
7	-0.051761	-2.310716	0.019134
6	1.119547	-2.995441	0.041347
6	2.331384	-2.373349	0.044689
1	1.056110	-4.087484	0.056144
1	3.256788	-2.941081	0.060982
6	-1.249772	-2.947301	0.003653
6	-2.436362	-2.277023	-0.015632
1	-1.230670	-4.041130	0.007829
1	-3.383546	-2.807610	-0.024131
15	2.315479	-0.582045	0.003252

15	-2.342936	-0.489088	-0.004301
6	3.360634	-0.103179	-1.449395
1	3.506302	0.981445	-1.492706
1	4.344120	-0.583900	-1.391085
1	2.854556	-0.426049	-2.362349
6	3.371591	-0.023516	1.418271
1	4.354431	-0.507673	1.382220
1	3.515415	1.061808	1.393652
1	2.871765	-0.291165	2.352424
6	-3.363415	0.103139	-1.431047
1	-4.379037	-0.306243	-1.381195
1	-3.424890	1.196475	-1.435343
1	-2.886692	-0.224832	-2.357955
6	-3.367371	0.059705	1.438887
1	-3.456533	1.150861	1.472047
1	-4.374453	-0.369517	1.381349
1	-2.881894	-0.279968	2.356866
77	-0.008226	-0.138307	-0.003774
6	1.241551	2.673996	0.028990
8	0.830733	4.018026	-0.201380
6	-0.513043	4.105056	0.259234
6	-1.130739	2.755434	-0.131393
6	0.021903	1.766661	-0.036419
1	2.002141	2.418845	-0.713988
1	1.691684	2.571021	1.032608
1	-0.544025	4.249146	1.352866
1	-0.979193	4.970427	-0.219587
1	-1.994717	2.467654	0.471474
1	-1.449646	2.782042	-1.183392
1	-0.009207	-0.368498	-1.664440
1	-0.012528	-0.332243	1.662066

Structure 23 - THF

B3LYP/GBS(1) = -1389.135899 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.428298 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.243726 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.509449 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.557924 a.u.
Enthalpy Correction = 0.363225
Gibbs Free Energy Correction = 0.293150

Atomic No	x-coord	y-coord	z-coord
7	-0.285128	-1.109074	1.472386
6	0.837979	-1.690712	1.975795
6	2.034129	-1.670223	1.319894
1	0.743193	-2.193874	2.943225
1	2.911673	-2.138764	1.756781
6	-1.510119	-1.262275	2.031860
6	-2.657193	-0.807295	1.439166
1	-1.555372	-1.778502	2.996141
1	-3.619975	-0.936087	1.925555
15	2.056193	-0.926199	-0.322047

15	-2.481932	-0.067726	-0.188059
6	2.368601	-2.310420	-1.515402
1	2.388026	-1.915634	-2.537031
1	3.324156	-2.803364	-1.302549
1	1.557518	-3.037738	-1.439529
6	3.663858	-0.024250	-0.474657
1	4.486977	-0.684359	-0.177100
1	3.814225	0.268179	-1.519794
1	3.652414	0.874529	0.142564
6	-3.465438	-1.077414	-1.383182
1	-4.514792	-1.146966	-1.074615
1	-3.411374	-0.625603	-2.379314
1	-3.033558	-2.079778	-1.431958
6	-3.467117	1.503829	-0.173708
1	-3.506237	1.928991	-1.182590
1	-4.491369	1.310648	0.164883
1	-3.010795	2.236536	0.497448
77	-0.152142	-0.086738	-0.432206
6	-0.043906	1.779058	0.934848
6	1.431233	2.787064	-0.591051
6	0.048607	2.204952	-0.387833
1	-0.954478	1.739040	1.521200
1	1.360065	3.885510	-0.688117
1	1.965243	2.400589	-1.464407
1	-0.778264	2.572528	-0.982283
1	-0.100036	0.331570	-1.997807
1	-0.401285	-1.529489	-1.111641
8	2.173264	2.439438	0.581316
6	1.267742	2.071066	1.625620
1	1.698194	1.227187	2.174094
1	1.136397	2.910280	2.332973

Structure 24 - THF

B3LYP/GBS(1) = -1389.133259 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.427094 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.247669 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.510120 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.55739 a.u.
Enthalpy Correction = 0.362570
Gibbs Free Energy Correction = 0.292908

Atomic No	x-coord	y-coord	z-coord
7	0.708702	2.023667	-0.000924
6	2.027543	2.349119	-0.001381
6	3.024942	1.420081	-0.000990
1	2.261464	3.416446	-0.002084
1	4.069882	1.713060	-0.001451
6	-0.255264	2.988782	-0.001211
6	-1.580492	2.699331	-0.000728
1	0.097368	4.022814	-0.001911
1	-2.326785	3.488298	-0.001077
15	2.482245	-0.280703	0.000303

15	-2.020020	0.955605	0.000437
6	3.293386	-1.128253	1.432362
1	3.049037	-2.196599	1.433876
1	4.383192	-1.021216	1.386369
1	2.923566	-0.681093	2.358269
6	3.293958	-1.130501	-1.430104
1	4.383709	-1.022981	-1.383945
1	3.050034	-2.198946	-1.429806
1	2.924328	-0.685098	-2.356938
6	-3.175098	0.749337	1.430855
1	-3.962445	1.510977	1.391753
1	-3.637598	-0.240542	1.397577
1	-2.614121	0.862992	2.362016
6	-3.177632	0.748406	-1.427756
1	-3.639802	-0.241569	-1.393151
1	-3.965054	1.509916	-1.387393
1	-2.618557	0.861904	-2.360087
77	0.151040	-0.004636	0.000056
6	-1.655809	-2.379923	-1.153379
8	-2.477988	-2.167597	-0.000838
6	-1.656079	-2.380907	1.151746
6	-0.246772	-2.034354	0.710698
6	-0.246599	-2.033847	-0.711708
1	-2.054567	-1.779495	-1.973380
1	-2.055057	-1.781154	1.972115
1	-1.690371	-3.444689	1.451073
1	0.577069	-2.404850	1.310304
1	0.577404	-2.403842	-1.311384
1	-1.690013	-3.443469	-1.453569
1	0.190203	0.182272	1.664572
1	0.190163	0.181817	-1.664434

Structure 25 - THF

B3LYP/GBS(1) = -231.211812 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -231.291746 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -231.139340 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -231.326701 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -231.285995 a.u.
Enthalpy Correction = 0.098319
Gibbs Free Energy Correction = 0.065527

Atomic No	x-coord	y-coord	z-coord
6	1.171616	-0.371707	0.000134
8	-0.000001	-1.189164	-0.000202
6	-1.171617	-0.371706	0.000071
6	-0.665597	1.045812	0.000016
6	0.665597	1.045811	-0.000073
1	1.785563	-0.600338	0.886690
1	1.785317	-0.600168	-0.886712
1	-1.785975	-0.600454	-0.886153

1	-1.784904	-0.600050	0.887249
1	-1.318096	1.912531	-0.000456
1	1.318097	1.912530	0.000107

Structure 26 - THF

B3LYP/GBS(1) = -1387.942824 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1388.225747 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1387.045371 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1388.302764 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1388.352492 a.u.
Enthalpy Correction = 0.345147
Gibbs Free Energy Correction = 0.275083

Atomic No	x-coord	y-coord	z-coord
7	0.686169	1.999894	-0.000950
6	2.011159	2.353862	-0.001962
6	3.020897	1.442606	-0.001955
1	2.227456	3.425426	-0.002915
1	4.062189	1.748403	-0.002944
6	-0.282800	2.977787	-0.001381
6	-1.605807	2.689588	-0.000910
1	0.071366	4.011870	-0.002229
1	-2.353647	3.477166	-0.001420
15	2.473709	-0.264433	0.000092
15	-2.021369	0.932756	0.000361
6	3.305859	-1.094870	1.434047
1	3.061563	-2.162956	1.447415
1	4.394689	-0.985570	1.374863
1	2.950864	-0.643778	2.364599
6	3.306596	-1.098784	-1.431102
1	4.395348	-0.988929	-1.371615
1	3.062712	-2.166998	-1.441442
1	2.951991	-0.650548	-2.363187
6	-3.182335	0.734969	1.431173
1	-3.975988	1.489327	1.382423
1	-3.632709	-0.260596	1.403435
1	-2.632012	0.860414	2.367656
6	-3.185260	0.733750	-1.427834
1	-3.635961	-0.261591	-1.397946
1	-3.978427	1.488556	-1.378199
1	-2.636913	0.857968	-2.365643
77	0.151938	-0.008116	0.000313
6	-1.624953	-2.372236	-1.154213
8	-2.452056	-2.173657	-0.000822
6	-1.624718	-2.373973	1.152129
6	-0.221908	-2.003769	0.711922
6	-0.222080	-2.002662	-0.713749
1	-2.035053	-1.772904	-1.972419
1	-2.034666	-1.775799	1.971270
1	-1.652124	-3.436427	1.458464
1	0.601467	-2.374295	1.318766
1	0.601180	-2.371979	-1.321476

1	-1.652309	-3.434249	-1.462082

Structure 27 - THF

B3LYP/GBS(1) = -1389.100421 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.394632 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.204921 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.474365 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.525293 a.u.
Enthalpy Correction = 0.361574
Gibbs Free Energy Correction = 0.289152

Atomic No	x-coord	y-coord	z-coord
7	-0.031443	-1.476818	1.381017
6	1.144923	-1.993336	1.835475
6	2.345845	-1.718342	1.255905
1	1.084550	-2.666291	2.695794
1	3.267473	-2.132201	1.654559
6	-1.227489	-1.976453	1.801262
6	-2.408198	-1.679223	1.191007
1	-1.200949	-2.654029	2.659659
1	-3.347008	-2.078255	1.563914
15	2.311031	-0.666368	-0.200018
15	-2.311525	-0.630532	-0.263273
6	2.993519	-1.635481	-1.619397
1	3.034698	-1.000796	-2.511099
1	3.999508	-2.009264	-1.396761
1	2.323824	-2.473665	-1.821039
6	3.701140	0.535573	0.062505
1	4.635975	-0.018649	0.206619
1	3.817845	1.194797	-0.803724
1	3.517975	1.144349	0.950789
6	-2.949149	-1.594462	-1.708058
1	-3.969331	-1.951333	-1.525655
1	-2.944447	-0.960756	-2.601558
1	-2.285404	-2.443293	-1.881611
6	-3.707826	0.581475	-0.075841
1	-3.743986	1.264578	-0.931197
1	-4.657095	0.035353	-0.026993
1	-3.595285	1.164908	0.839694
77	-0.000433	-0.183196	-0.331247
6	1.164062	2.687822	0.046540
8	0.661805	4.019986	-0.018413
6	-0.513316	4.018727	0.780123
6	-1.153186	2.646666	0.508289
6	0.004405	1.719917	0.169647
1	1.789897	2.510623	-0.830286
1	1.794057	2.564443	0.948975
1	-0.258806	4.127774	1.848915
1	-1.129789	4.871122	0.481719
1	-1.752263	2.265242	1.339904
1	-1.808435	2.699718	-0.371051
1	-0.021296	-1.632705	-1.179295

1	0.046345	0.358478	-1.859420

Structure 27-28TS - THF

B3LYP/GBS(1) = -1389.071124 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.368339 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1388.175015 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1389.447210 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1389.501476 a.u.
Enthalpy Correction = 0.357914
Gibbs Free Energy Correction = 0.285760
Imaginary Freq = -840.9 i

Atomic No	x-coord	y-coord	z-coord
7	-0.008443	-2.102325	-0.740364
6	1.170211	-2.719553	-1.005239
6	2.372869	-2.164870	-0.687736
1	1.119739	-3.699755	-1.489136
1	3.305652	-2.667503	-0.926013
6	-1.197416	-2.708184	-0.987434
6	-2.391099	-2.143851	-0.654553
1	-1.162401	-3.689632	-1.470136
1	-3.329774	-2.642529	-0.878076
15	2.338093	-0.548716	0.087036
15	-2.340885	-0.528443	0.122709
6	3.522137	0.455667	-0.929219
1	3.790040	1.393296	-0.434994
1	4.435531	-0.127299	-1.094050
1	3.067409	0.679860	-1.897745
6	3.281076	-0.685204	1.676391
1	4.289049	-1.079087	1.502951
1	3.360090	0.297626	2.153652
1	2.745348	-1.359505	2.349506
6	-3.588593	0.458222	-0.835422
1	-4.523715	-0.110841	-0.894612
1	-3.793818	1.420843	-0.358484
1	-3.221818	0.631718	-1.850604
6	-3.223698	-0.674551	1.746264
1	-3.304669	0.309690	2.220287
1	-4.229590	-1.087188	1.608639
1	-2.653090	-1.335188	2.403850
77	0.007080	-0.146829	0.258425
6	0.035731	1.721513	-0.194368
6	0.564135	4.074739	-0.048044
6	1.210303	2.698490	-0.246708
1	1.113812	4.902326	-0.506679
1	0.431761	4.295979	1.025854
1	1.668579	2.656547	-1.244849
1	1.985882	2.476016	0.489988
1	0.010940	-0.232598	1.931552
1	-0.019213	-1.240757	1.694380
8	-0.691472	3.963816	-0.702866
6	-1.159825	2.639109	-0.449270

1	-1.749935	2.333315	-1.316911
1	-1.823193	2.634474	0.434182

Structure 28 - THF

B3LYP/GBS(1) = -1387.921871 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1388.204558 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1387.015494 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1388.278016 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1388.331148 a.u.
Enthalpy Correction = 0.344487
Gibbs Free Energy Correction = 0.271707

Atomic No	x-coord	y-coord	z-coord
7	0.025799	-2.268566	-0.018317
6	-1.156782	-2.965040	-0.040213
6	-2.364930	-2.345698	-0.044644
1	-1.087863	-4.056581	-0.053602
1	-3.291662	-2.911119	-0.060686
6	1.221477	-2.941963	0.002287
6	2.418232	-2.299835	0.024174
1	1.173622	-4.034722	0.000371
1	3.355326	-2.847860	0.036312
15	-2.313474	-0.546250	-0.004849
15	2.326707	-0.502949	0.008186
6	-3.362111	-0.073886	1.450640
1	-3.493096	1.012138	1.499810
1	-4.349934	-0.544468	1.385268
1	-2.867451	-0.407070	2.366974
6	-3.376372	0.004134	-1.421223
1	-4.366876	-0.462496	-1.369370
1	-3.497105	1.092291	-1.410510
1	-2.894389	-0.284247	-2.359308
6	3.357792	0.066183	1.440042
1	4.369263	-0.352692	1.386367
1	3.426320	1.158825	1.450274
1	2.883485	-0.261656	2.368977
6	3.374750	0.011666	-1.433908
1	3.473899	1.101304	-1.476837
1	4.375827	-0.428903	-1.361084
1	2.899722	-0.331511	-2.356890
77	0.006646	-0.151287	0.000134
6	-1.207028	2.676292	0.000113
8	-0.781572	4.020112	0.215716
6	0.555458	4.093295	-0.265514
6	1.165030	2.733339	0.100044
6	0.000631	1.751152	0.031954
1	-1.950702	2.433024	0.766199
1	-1.695077	2.580419	-0.988736
1	0.569465	4.247326	-1.358764
1	1.039329	4.951016	0.210767
1	2.006123	2.444085	-0.535918
1	1.526628	2.751221	1.139967

3.3. Coordinates of THF structures at the Full-opt level of theory

Full Structure 5 - THF
B3LYP/GBS(1) = -2089.541867 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2090.023289 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2090.023289 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -2084.982603 a.u.
Enthalpy Correction = 0.765571
Gibbs Free Energy Correction = 0.648863

Atomic No	x-coord	y-coord	z-coord
1	5.871048	4.136815	0.761237
1	6.431156	2.591083	0.105781
6	5.705423	3.399790	-0.034306
1	5.949447	3.895083	-0.984262
1	3.355772	4.796549	0.278846
6	3.187719	3.732867	0.118080
6	4.288680	2.876360	-0.022763
1	3.056515	0.380294	2.724411
1	3.059530	-1.124956	3.661377
1	5.136953	-0.551182	1.495909
1	1.074448	3.980421	0.198130
6	1.879162	3.270010	0.059987
6	4.004220	1.513733	-0.131483
1	4.836861	0.817376	-0.192221
6	2.675719	-0.646532	2.751599
1	5.009278	-2.061046	2.397181
1	-2.133450	0.974325	4.200408
6	4.670054	-1.540842	1.492412
1	1.585502	-0.602736	2.817673
1	-1.704284	1.947300	2.779607
1	-0.783789	0.482885	3.156225
6	-1.785515	0.924769	3.160875
6	2.694472	1.014036	-0.148570
6	1.578742	1.900185	-0.147599
1	5.054186	-2.098337	0.632858
6	3.136124	-1.436595	1.515352
1	0.122627	3.717807	-1.694078
1	-4.260067	5.634582	-0.136514
1	2.720995	-2.451351	1.587580
1	-1.839501	5.147611	-1.899614
6	-0.796809	3.414413	-1.207687
7	0.284848	1.373384	-0.266197
6	-1.921557	4.221497	-1.333218
15	2.301867	-0.769244	-0.041869
6	-0.832201	2.200480	-0.481384
1	-3.250225	-1.263132	3.956533
6	-2.760566	0.079616	2.326392
1	4.287777	-1.210706	-1.355482
1	-3.739727	0.578330	2.334049
6	-3.152216	3.873677	-0.757860

6	-4.349189	4.791745	-0.835724
1	-1.961522	-1.870807	2.892773
6	-2.109357	1.779706	-0.019304
1	-4.466000	5.220099	-1.838732
6	-2.913566	-1.333010	2.914232
6	-3.218566	2.628193	-0.127896
77	-0.031316	-0.681592	0.112731
6	3.248789	-1.547523	-1.469814
1	-5.276002	4.262245	-0.589462
1	-4.172625	2.301334	0.278026
1	2.762466	0.077087	-2.857368
15	-2.214525	0.034374	0.531926
1	3.665236	-3.486075	-0.507535
1	-3.638299	-1.942421	2.366057
6	2.723324	-1.015740	-2.813026
6	3.229851	-3.084091	-1.427974
1	3.333541	-1.410453	-3.635244
1	3.808754	-3.485380	-2.269364
1	1.687056	-1.325327	-2.985459
1	2.210790	-3.471701	-1.511238
1	-5.173636	-0.817159	1.146074
1	-5.361624	0.537842	0.018308
6	-3.635842	-0.747334	-0.434244
6	-5.056900	-0.510751	0.102716
1	-3.394613	-1.811311	-0.331761
1	-3.848274	0.673529	-2.084704
1	-2.545827	-0.495049	-2.327621
6	-3.554743	-0.368598	-1.922990
1	-5.767927	-1.099799	-0.491104
1	-4.233231	-1.005443	-2.504436
6	-1.932006	-4.443339	-0.306707
6	-1.657648	-4.212470	-1.810133
6	-0.696718	-2.990525	-1.809755
6	-0.431867	-2.704356	-0.311287
8	-1.627272	-3.213869	0.338833
1	-2.971972	-4.700063	-0.079416
1	-1.212856	-5.096770	-2.279018
1	0.230120	-3.192553	-2.355829
1	0.393207	-3.357862	0.019581
1	-1.285692	-5.247754	0.084073
1	-2.583125	-3.987543	-2.350994
1	-1.169733	-2.129456	-2.292575
1	-0.045915	-1.489592	1.455373

Full Structure 5-6TS – THF (Note; All efforts to fully converge this failed. The result presented here is the closest approximation)

B3LYP/GBS(1) = -2089.517304 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2090.003020 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2088.872196 a.u.
Enthalpy Correction = 0.759924
Gibbs Free Energy Correction = 0.644889
Imaginary Freq = -851.4 i

Atomic No	x-coord	y-coord	z-coord
1	-6.164255	2.971179	-0.714863
1	-5.504981	4.576420	-0.379875
6	-5.382784	3.681787	-1.005690
1	-5.583334	3.988494	-2.040604
1	-2.967654	4.703452	-1.826407
6	-2.858316	3.749266	-1.313112
6	-4.006611	3.076676	-0.857950
1	-3.642029	-0.368820	-2.320970
1	-3.864849	-2.111060	-2.564667
1	-5.428318	-0.561674	-0.423614
1	-0.733196	3.775188	-1.520467
6	-1.586808	3.230398	-1.133740
6	-3.811188	1.820674	-0.285621
1	-4.683970	1.269070	0.051371
6	-3.287771	-1.358051	-2.012662
1	-5.495662	-2.305430	-0.655737
1	2.706017	0.388396	-3.950092
6	-4.964199	-1.505440	-0.124067
1	-2.237613	-1.441671	-2.309705
1	2.094842	1.480773	-2.693350
1	1.226819	-0.019904	-3.054118
6	2.221804	0.429365	-2.965895
6	-2.537453	1.248222	-0.130193
6	-1.370906	1.986449	-0.478700
1	-5.142724	-1.652717	0.945392
6	-3.472537	-1.561799	-0.499446
1	-0.013849	4.095453	0.526349
1	5.519522	3.938592	0.810174
1	-3.123780	-2.569457	-0.251190
1	2.004909	5.379243	0.929924
6	0.944046	3.603930	0.408476
7	-0.123568	1.450598	-0.229491
6	2.099009	4.331038	0.649489
15	-2.269292	-0.456325	0.466790
6	0.984463	2.228384	0.047334
1	3.870888	-1.751316	-3.360997
6	3.076847	-0.328353	-1.936918
1	-3.995979	-0.269244	2.160104
1	4.042839	0.189275	-1.851491
6	3.377947	3.757547	0.553382
6	4.629154	4.575846	0.769029
1	2.388928	-2.299703	-2.561384
6	2.275719	1.621625	0.056313
1	4.786814	5.304914	-0.037887
6	3.332215	-1.768108	-2.404715
6	3.428180	2.393565	0.267820
77	0.052024	-0.715743	0.109862
6	-2.924742	-0.500147	2.229523
1	4.586486	5.144906	1.706887
1	4.401861	1.914860	0.215233
1	-2.405004	1.577107	2.686427
15	2.312347	-0.180786	-0.217506
1	-3.279965	-2.674620	2.280579
1	3.929092	-2.348034	-1.694020
6	-2.267518	0.575793	3.105522
6	-2.750688	-1.897680	2.845056
1	-2.716904	0.559902	4.106723
1	-3.142687	-1.912537	3.869741
1	-1.192719	0.398461	3.209385
1	-1.688930	-2.166859	2.885975

1	5.321423	-0.992770	-0.362018
1	5.363332	0.239058	0.911780
6	3.544637	-0.992834	0.955066
6	5.042523	-0.779910	0.674358
1	3.319991	-2.054505	0.798224
1	3.371875	0.413894	2.621453
1	2.170478	-0.886570	2.653451
6	3.210931	-0.650296	2.416119
1	5.625855	-1.454824	1.314038
1	3.859879	-1.226387	3.088140
6	1.345229	-4.592084	-0.765061
6	0.025278	-5.071068	-0.170767
6	-0.807480	-3.777112	-0.194334
6	0.224932	-2.632886	-0.165820
8	1.451241	-3.222274	-0.323249
1	2.231947	-5.118553	-0.405377
1	-0.426631	-5.887739	-0.741233
1	-1.413868	-3.714471	-1.102866
1	1.337959	-4.611340	-1.863739
1	0.178563	-5.415648	0.857571
1	-1.480658	-3.701070	0.661728
1	0.243987	-0.145264	1.608653
1	-0.054872	-1.722371	-1.415637

Full Structure 5-7TS - THF

B3LYP/GBS(1) = -2089.499594 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2089.988111 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2088.857831 a.u.
Enthalpy Correction = 0.761129
Gibbs Free Energy Correction = 0.646209
Imaginary Freq = -115.4 i

Atomic No	x-coord	y-coord	z-coord
1	-5.551977	4.015952	-2.001201
1	-6.148110	3.002596	-0.678663
6	-5.353762	3.698695	-0.969238
1	-5.453628	4.591591	-0.337112
1	-2.928568	4.652519	-1.842166
6	-2.832895	3.705928	-1.312856
6	-3.989682	3.064778	-0.832283
1	-3.208723	-0.318526	-2.493034
1	-3.458995	-2.043717	-2.817730
1	-5.267715	-0.482041	-0.894475
1	-0.710142	3.688429	-1.540841
6	-1.569791	3.165790	-1.137922
6	-3.813953	1.812143	-0.248952
1	-4.692490	1.276988	0.100230
6	-2.943884	-1.329154	-2.163061
1	-5.368882	-2.218371	-1.175249
1	2.499694	0.277996	-3.953028
6	-4.892683	-1.450471	-0.552022
1	-1.864129	-1.453485	-2.289039

1	1.719035	1.266977	-2.704941
1	1.155924	-0.385394	-2.995095
6	2.044821	0.253013	-2.954554
6	-2.547790	1.219701	-0.097314
6	-1.375115	1.934160	-0.456133
1	-5.234330	-1.610138	0.475786
6	-3.365994	-1.558819	-0.702941
1	-0.062767	4.043838	0.550343
1	4.690160	5.366049	-0.134044
1	-3.089342	-2.582562	-0.431906
1	1.931884	5.381501	0.904846
6	0.904649	3.575907	0.417398
7	-0.125027	1.395792	-0.196547
6	2.046651	4.334580	0.628414
15	-2.294723	-0.497067	0.447188
6	0.979235	2.203722	0.066634
1	4.105152	-1.556080	-3.338178
6	3.056726	-0.294500	-1.934971
1	-4.177718	-0.416518	1.979193
1	3.904586	0.404005	-1.888254
6	3.335609	3.791925	0.506094
6	4.570377	4.643494	0.684843
1	2.759694	-2.372669	-2.509860
6	2.277344	1.625865	0.055187
1	4.532706	5.222344	1.616660
6	3.581467	-1.667366	-2.379584
6	3.415415	2.426736	0.230311
77	0.048925	-0.657842	0.248620
6	-3.117188	-0.657263	2.131863
1	5.477276	4.029618	0.713211
1	4.399160	1.973037	0.155680
1	-2.635925	1.380036	2.771087
15	2.314392	-0.179696	-0.198864
1	-3.476898	-2.827346	1.998628
1	4.286952	-2.106392	-1.666830
6	-2.539564	0.352213	3.133930
6	-3.008060	-2.094449	2.665295
1	-3.076779	0.274704	4.087820
1	-3.502740	-2.174535	3.641240
1	-1.478197	0.160410	3.320436
1	-1.957498	-2.377281	2.799991
1	5.362771	-0.642445	-0.300450
1	5.273915	0.365103	1.155699
6	3.566891	-0.989310	0.948978
6	5.048870	-0.624809	0.747268
1	3.435302	-2.047981	0.689901
1	3.208404	0.253419	2.711027
1	2.153472	-1.161911	2.615091
6	3.167246	-0.802926	2.421875
1	5.674799	-1.344947	1.289709
1	3.862903	-1.355828	3.066198
6	1.482295	-4.559134	-0.707977
6	0.157369	-4.985872	-0.074377
6	-0.749976	-3.791637	-0.419704
6	0.194353	-2.589864	-0.398088
8	1.451475	-3.116127	-0.751968
1	2.363651	-4.871269	-0.136751
1	-0.206434	-5.942167	-0.462861
1	-1.164338	-3.909572	-1.430245
1	1.586078	-4.932274	-1.735480
1	0.261312	-5.078452	1.013347

1	-1.581736	-3.689517	0.278044
1	0.211740	0.069966	1.691246
1	0.268715	-2.310412	0.878286

Full Structure 5-9TS – THF (Note; All efforts to fully converge this failed due to a flat surface at the transition point. The transition structure and agostic C-H-Ir minimum are very close energetically and structurally and neither stationary point converge. The structure presented here is a very close approximation.)
B3LYP/GBS(1) = -2089.48519778 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2089.974958 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2088.848314 a.u.
Enthalpy Correction = 0.763491
Gibbs Free Energy Correction = 0.650595

Atomic No	x-coord	y-coord	z-coord
1	5.336951	4.557126	0.929643
1	6.102300	3.078575	0.329815
6	5.308502	3.806582	0.129440
1	5.569645	4.325606	-0.803173
1	2.814141	4.964633	0.139196
6	2.766096	3.882285	0.029892
6	3.957891	3.136976	0.040835
1	3.312216	0.483058	2.706661
1	3.403750	-1.021642	3.641673
1	5.300858	-0.478162	1.303768
1	0.644177	3.920170	-0.071220
6	1.521788	3.288155	-0.102845
6	3.819894	1.752378	-0.012559
1	4.716797	1.140092	0.038800
6	2.937937	-0.544480	2.770267
1	5.214848	-1.935971	2.288988
1	-2.089774	1.313567	4.201495
6	4.822650	-1.459913	1.381539
1	1.859370	-0.501340	2.932648
1	-2.103715	2.182284	2.654532
1	-0.745522	1.118817	3.058919
6	-1.830466	1.239609	3.137520
6	2.570151	1.119399	-0.114066
6	1.373534	1.880450	-0.248522
1	5.147115	-2.066350	0.531975
6	3.292396	-1.337843	1.502296
1	-0.214323	3.407505	-2.028462
1	-4.572202	5.270566	-0.446295
1	2.880966	-2.351544	1.613947
1	-2.267132	4.716242	-2.225639
6	-1.090522	3.103163	-1.467170
7	0.161799	1.231634	-0.445973
6	-2.260887	3.838709	-1.581451
15	2.362623	-0.679969	-0.019758

6	-1.018194	1.949339	-0.646538
1	-2.580579	-1.161256	4.321947
6	-2.567480	0.045838	2.514590
1	4.407714	-0.981488	-1.256027
1	-3.643740	0.245544	2.579466
6	-3.436010	3.476499	-0.899855
6	-4.685886	4.320333	-0.985584
1	-1.178824	-1.446885	3.269758
6	-2.235107	1.508032	-0.067151
1	-4.934514	4.571373	-2.024484
6	-2.256003	-1.252734	3.277703
6	-3.396077	2.290365	-0.168124
77	0.010569	-0.773633	0.148111
6	3.387940	-1.328213	-1.470525
1	-5.548475	3.801374	-0.553796
1	-4.303961	1.952969	0.328027
1	3.070516	0.410432	-2.755384
15	-2.191129	-0.153727	0.676904
1	3.720227	-3.340826	-0.627054
1	-2.753554	-2.129898	2.849025
6	2.960503	-0.676836	-2.796329
6	3.425179	-2.864165	-1.568021
1	3.591665	-1.051819	-3.612338
1	4.152996	-3.168575	-2.330852
1	1.918161	-0.894698	-3.045446
1	2.455462	-3.276859	-1.860572
1	-4.726033	-1.666108	1.854300
1	-5.376497	-0.210299	1.077349
6	-3.690328	-1.105128	-0.014147
6	-4.931961	-1.194909	0.889553
1	-3.280851	-2.115457	-0.115876
1	-4.758307	0.279228	-1.326149
1	-3.261732	-0.308306	-2.032418
6	-4.110028	-0.598083	-1.408072
1	-5.695740	-1.802178	0.386654
1	-4.673499	-1.380991	-1.931093
6	-1.872864	-3.961830	-1.539595
6	-1.439164	-2.706265	-2.317068
6	-0.198277	-2.229681	-1.542381
6	-0.160467	-3.074832	-0.313606
8	-1.371845	-3.787472	-0.198209
1	-2.955151	-4.104392	-1.461285
1	-1.190763	-2.956185	-3.355621
1	0.702550	-2.282818	-2.142318
1	0.715410	-3.714770	-0.147764
1	0.284402	-0.159835	1.645209
1	-0.124482	-2.450279	0.777607
1	-1.434027	-4.874882	-1.970341
1	-2.241324	-1.971055	-2.352252

Full Structure 5-10TS - THF

B3LYP/GBS(1) = -2089.497509 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2089.986520 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2088.86235 a.u.

Enthalpy Correction = 0.760414
Gibbs Free Energy Correction = 0.648109
Imaginary Freq = -810.1 i

Atomic No	x-coord	y-coord	z-coord
1	-5.837450	3.383952	-2.333778
1	-6.388238	2.407787	-0.964964
6	-5.652301	3.157329	-1.275745
1	-5.862586	4.076367	-0.712110
1	-3.293316	4.334244	-2.042653
6	-3.130592	3.411063	-1.488674
6	-4.240987	2.670025	-1.046506
1	-4.193215	-0.850591	-1.941875
1	-4.053875	-2.606257	-2.142731
1	-5.429771	-1.112639	0.352071
1	-1.005851	3.588916	-1.635891
6	-1.829187	2.996802	-1.252779
6	-3.973765	1.460851	-0.405524
1	-4.813606	0.854550	-0.076457
6	-3.576034	-1.721772	-1.703007
1	-5.390243	-2.835894	-0.019612
1	3.055836	0.344980	-3.871683
6	-4.835974	-2.024712	0.469593
1	-2.608336	-1.573922	-2.191227
1	1.962837	1.222060	-2.783758
1	1.646500	-0.472501	-3.165320
6	2.441209	0.255100	-2.966817
6	-2.666681	1.000728	-0.182000
6	-1.546093	1.794801	-0.551234
1	-4.786109	-2.261457	1.536105
6	-3.445379	-1.902243	-0.179135
1	-0.357337	3.984934	0.445962
1	4.308955	5.570156	-0.054948
1	-2.924480	-2.851516	0.008543
1	1.559526	5.420485	0.849197
6	0.636073	3.562728	0.354343
7	-0.266813	1.342021	-0.278830
6	1.731493	4.376256	0.592089
15	-2.260497	-0.616856	0.554395
6	0.782100	2.187902	0.018028
1	4.702373	-1.338568	-2.963498
6	3.314308	-0.176911	-1.778782
1	-3.835061	-0.411106	2.381378
1	4.063987	0.609667	-1.619019
6	3.048863	3.893183	0.515678
6	4.236530	4.802317	0.727363
1	3.389353	-2.307102	-2.300569
6	2.108928	1.668546	0.060435
1	4.178390	5.331971	1.687500
6	4.068477	-1.480700	-2.078759
6	3.199296	2.531493	0.259148
77	0.025158	-0.784651	0.039996
6	-2.741820	-0.510477	2.368386
1	5.175627	4.238187	0.719277
1	4.205924	2.127165	0.220474
1	-2.472828	1.655042	2.542918
15	2.299929	-0.135040	-0.175626
1	-2.781141	-2.694082	2.686339
1	4.717930	-1.794407	-1.256395

6	-2.145678	0.735918	3.037829
6	-2.341174	-1.789019	3.121623
1	-2.469020	0.778603	4.085595
1	-2.674306	-1.730705	4.165271
1	-1.051694	0.709424	3.018114
1	-1.252530	-1.907568	3.120594
1	5.362051	-0.131905	0.153208
1	4.928825	0.720206	1.644769
6	3.487357	-0.838216	1.115339
6	4.912034	-0.252208	1.143403
1	3.543826	-1.888932	0.806822
1	2.670997	0.210282	2.853939
1	1.968337	-1.394013	2.582950
6	2.890153	-0.813830	2.530115
1	5.563021	-0.922660	1.718797
1	3.613044	-1.243532	3.235726
6	1.757513	-4.155338	-0.825152
6	0.279070	-2.863426	0.368649
6	-0.179528	-2.782716	-1.008924
1	2.823132	-4.184300	-1.070727
1	-0.347616	-3.304334	1.143416
1	-1.210906	-3.016626	-1.241468
1	-0.252974	-1.269966	-1.602933
1	0.286952	-0.303866	1.575432
1	1.411167	-5.190197	-0.670449
8	1.597649	-3.404318	0.381910
6	0.885003	-3.450260	-1.885287
1	1.446792	-2.729172	-2.480767
1	0.425648	-4.163485	-2.578453

Full Structure 6 - THF

B3LYP/GBS(1) = -2089.542305 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2090.027357 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2088.890988 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -2084.994473 a.u.
Enthalpy Correction = 0.761519
Gibbs Free Energy Correction = 0.645917

Atomic No	x-coord	y-coord	z-coord
1	-5.337369	4.220343	-2.083947
1	-6.056752	3.092882	-0.926135
6	-5.250598	3.821851	-1.064569
1	-5.444714	4.658127	-0.379026
1	-2.760865	4.904622	-1.491957
6	-2.707437	3.900837	-1.072924
6	-3.897236	3.196562	-0.820826
1	-3.787945	-0.203565	-2.347166
1	-3.994618	-1.933512	-2.678232
1	-5.480482	-0.526133	-0.325064
1	-0.574587	3.931169	-1.053441
6	-1.460412	3.354415	-0.814951
6	-3.762655	1.888963	-0.354840
1	-4.665347	1.312328	-0.176177
6	-3.405932	-1.201707	-2.110066
1	-5.550846	-2.235446	-0.741384
1	2.646303	0.677789	-4.039134
6	-4.995579	-1.491912	-0.154998
1	-2.367236	-1.250695	-2.448426

1	2.292711	1.746013	-2.667325
1	1.159278	0.452130	-3.091293
6	2.219912	0.716002	-3.028436
6	-2.513511	1.294999	-0.120045
6	-1.314261	2.045470	-0.279802
1	-5.118981	-1.752151	0.900414
6	-3.523117	-1.498309	-0.605730
1	0.121390	3.978518	1.041688
1	4.888454	5.190856	0.248105
1	-3.150808	-2.515825	-0.442565
1	2.199580	5.187395	1.425548
6	1.060147	3.496473	0.795008
7	-0.105030	1.451650	0.019161
6	2.246008	4.177014	1.021873
15	-2.296692	-0.444992	0.387854
6	1.045881	2.171841	0.280685
1	3.417009	-1.670492	-3.702530
6	2.974485	-0.260905	-2.114261
1	-4.011882	-0.239849	2.090992
1	4.014872	0.082632	-2.033295
6	3.499576	3.598606	0.759033
6	4.781652	4.369195	0.969719
1	1.933304	-2.042668	-2.803545
6	2.314948	1.551277	0.106640
1	4.826270	4.817944	1.970597
6	2.961439	-1.679558	-2.704095
6	3.497804	2.276710	0.314188
77	0.024268	-0.721667	-0.001230
6	-2.946705	-0.499000	2.157606
1	5.658646	3.722033	0.858957
1	4.453814	1.793057	0.132629
1	-2.404715	1.566415	2.640140
15	2.286846	-0.212811	-0.361418
1	-3.341702	-2.668163	2.216230
1	3.513000	-2.399139	-2.090033
6	-2.252838	0.556412	3.031449
6	-2.807860	-1.895098	2.782016
1	-2.663597	0.519257	4.048677
1	-3.216967	-1.895610	3.800125
1	-1.175459	0.371095	3.086698
1	-1.751067	-2.178625	2.847690
1	5.179048	-1.375706	-0.782468
1	5.437869	-0.025059	0.334494
6	3.562916	-1.122030	0.701193
6	5.031547	-1.037862	0.247466
1	3.242767	-2.163835	0.595336
1	3.761066	0.292314	2.358669
1	2.391434	-0.816641	2.524518
6	3.426781	-0.735465	2.183064
1	5.641920	-1.682749	0.892997
1	4.047791	-1.402587	2.794925
6	1.263333	-4.700444	-0.341031
6	-0.042456	-5.016584	0.380283
6	-0.851715	-3.741325	0.100757
6	0.187796	-2.634318	-0.053745
8	1.363512	-3.251801	-0.289185
1	2.162519	-5.103025	0.130251
1	-0.518706	-5.928317	0.009459
1	-1.393542	-3.819414	-0.852086
1	1.247764	-4.997208	-1.396482
1	0.132083	-5.132977	1.455477

1	-1.578148	-3.505710	0.877508
1	0.328943	-0.594618	1.646230
1	-0.296857	-0.581641	-1.643044

Full Structure 7 - THF

B3LYP/GBS(1) = -2089.534335 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2090.018838 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2088.886760 a.u.
Enthalpy Correction = 0.762555
Gibbs Free Energy Correction = 0.648521

Atomic No	x-coord	y-coord	z-coord
1	5.251017	4.671384	0.162437
1	5.972332	3.123789	-0.301807
6	5.153370	3.817955	-0.520798
1	5.316721	4.204077	-1.536725
1	2.658137	4.968350	-0.410649
6	2.612544	3.880848	-0.371984
6	3.809327	3.143031	-0.383233
1	3.400802	1.136140	2.624321
1	3.337518	-0.076746	3.917981
1	5.272791	-0.269184	1.438927
1	0.489356	3.901977	-0.252668
6	1.369598	3.273301	-0.301085
6	3.685280	1.762885	-0.235331
1	4.593030	1.164563	-0.182857
6	2.934628	0.194789	2.933985
1	5.153566	-1.318640	2.849913
1	-1.766702	1.714208	4.198185
6	4.757020	-1.148611	1.840982
1	1.860871	0.363263	3.039655
1	-1.828165	2.274758	2.516189
1	-0.507537	1.220489	3.045513
6	-1.576114	1.424581	3.156950
6	2.442909	1.115622	-0.130128
6	1.220780	1.856536	-0.245598
1	5.033685	-2.015937	1.235029
6	3.236829	-0.930066	1.931083
1	-0.565780	3.272752	-1.916498
1	-5.325714	4.383861	-0.900782
1	2.773274	-1.851887	2.304573
1	-2.773759	4.178421	-2.371360
6	-1.417444	2.845194	-1.401259
7	0.014616	1.189705	-0.221038
6	-2.681906	3.348044	-1.672655
15	2.322934	-0.658950	0.286499
6	-1.215015	1.753605	-0.512835
1	-2.336310	-0.633399	4.818565
6	-2.412823	0.185811	2.809347
1	4.423018	-1.309006	-0.751235

1	-3.471646	0.470915	2.867868
6	-3.839466	2.809419	-1.089116
6	-5.205842	3.393419	-1.360897
1	-1.101420	-1.289923	3.721825
6	-2.402854	1.149989	0.015545
1	-5.388348	3.518886	-2.436035
6	-2.144778	-0.965868	3.790496
6	-3.663013	1.700595	-0.258893
77	0.015815	-0.934529	0.381235
6	3.383424	-1.590338	-0.960191
1	-5.999878	2.751771	-0.963431
1	-4.544842	1.245452	0.183314
1	3.177431	-0.111175	-2.563811
15	-2.151080	-0.360692	1.028013
1	3.485602	-3.427522	0.252441
1	-2.780455	-1.838318	3.601033
6	3.080720	-1.189720	-2.408759
6	3.221260	-3.106980	-0.760945
1	3.778490	-1.698048	-3.086555
1	3.867555	-3.652005	-1.461116
1	2.068884	-1.488621	-2.696467
1	2.183452	-3.406238	-0.939995
1	-4.808130	-1.204276	2.522294
1	-5.400108	-0.416860	1.051065
6	-3.562397	-1.592647	0.741518
6	-4.906299	-1.313563	1.439117
1	-3.138909	-2.502999	1.186972
1	-4.120314	-0.979859	-1.285675
1	-2.860029	-2.232486	-1.220443
6	-3.778382	-1.873665	-0.752480
1	-5.584490	-2.157445	1.258652
1	-4.541475	-2.652168	-0.876816
6	-0.772120	-2.998512	-3.276945
6	-0.581735	-1.626455	-3.923811
6	-0.665462	-0.681906	-2.710681
6	-0.359484	-1.537526	-1.491226
8	-0.411496	-2.812128	-1.870216
1	-1.810920	-3.344444	-3.295483
1	0.399295	-1.558028	-4.404889
1	0.007307	0.176523	-2.757064
1	-0.126825	-3.788890	-3.665591
1	-1.341484	-1.420674	-4.682578
1	-1.672594	-0.266445	-2.573565
1	0.025003	-2.472216	0.869765
1	0.325460	-0.534276	1.962772

Full Structure 7-8TS - THF

B3LYP/GBS(1) = -2089.489659 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2089.977261 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2088.846383 a.u.
Enthalpy Correction = 0.758565
Gibbs Free Energy Correction = 0.645192
Imaginary Freq = -953.6 i

Atomic No	x-coord	y-coord	z-coord
1	-5.046063	3.906237	-1.605479
1	-5.725695	2.940728	-0.287553
6	-4.886256	3.586776	-0.567458
1	-4.947165	4.489694	0.055692
1	-2.395980	4.371281	-1.429666
6	-2.364955	3.433518	-0.876929
6	-3.564488	2.875372	-0.398825
1	-2.785200	-0.619692	-1.997963
1	-3.186616	-2.321243	-2.294064
1	-4.969779	-0.520494	-0.606648
1	-0.245857	3.283322	-1.073030
6	-1.139852	2.823445	-0.668225
6	-3.471037	1.628804	0.216470
1	-4.386110	1.158795	0.565766
6	-2.654492	-1.639020	-1.618541
1	-5.226819	-2.251533	-0.818930
1	2.440661	-0.402229	-3.367239
6	-4.730775	-1.502135	-0.188513
1	-1.586234	-1.873062	-1.652503
1	2.050186	0.773104	-2.097841
1	1.049014	-0.672855	-2.295442
6	2.074958	-0.292937	-2.338044
6	-2.246437	0.962096	0.401169
6	-1.023591	1.596881	0.045603
1	-5.176915	-1.571461	0.808943
6	-3.215535	-1.766770	-0.192736
1	0.494292	3.661750	0.940780
1	5.388971	4.435981	0.282013
1	-3.068914	-2.799711	0.137932
1	2.610910	4.805788	1.268042
6	1.410646	3.093075	0.842927
7	0.177659	0.988767	0.339534
6	2.621486	3.740553	1.041776
15	-2.146737	-0.756780	1.010497
6	1.344976	1.703162	0.558030
1	3.547019	-2.572183	-2.840203
6	2.988249	-1.077743	-1.382709
1	-4.142862	-0.418053	2.350353
1	3.987881	-0.621562	-1.418470
6	3.849868	3.064862	0.973744
6	5.162573	3.792730	1.143732
1	2.109739	-3.001250	-1.895655
6	2.584024	0.999498	0.589110
1	5.156121	4.440031	2.030107
6	3.098546	-2.539523	-1.838700
6	3.793341	1.686862	0.758925
77	0.189669	-1.136335	1.007657
6	-3.138392	-0.774459	2.613514
1	5.996609	3.090704	1.253260
1	4.726240	1.131534	0.737705
1	-2.474890	1.211970	3.251459
15	2.450340	-0.813153	0.412611
1	-3.752474	-2.886930	2.498125
1	3.714633	-3.152851	-1.174528
6	-2.552337	0.195655	3.649085
6	-3.256139	-2.195025	3.188133
1	-3.197796	0.223753	4.536223
1	-3.841905	-2.180833	4.115800
1	-1.552620	-0.116973	3.967079
1	-2.266214	-2.601642	3.426796

1	5.313001	-1.965914	-0.095034
1	5.670251	-0.632006	1.011708
6	3.774086	-1.657477	1.460873
6	5.223086	-1.628250	0.940998
1	3.429867	-2.697922	1.430994
1	4.011869	-0.132306	3.013996
1	2.702496	-1.277837	3.334176
6	3.710006	-1.180931	2.921223
1	5.837089	-2.297595	1.557501
1	4.389469	-1.784259	3.536544
6	1.242476	-5.124067	0.262992
6	-0.114025	-5.417552	0.892490
6	-0.863170	-4.109589	0.591794
6	0.215910	-3.024754	0.571678
8	1.402961	-3.695180	0.404842
1	2.092381	-5.600329	0.758461
1	-0.595056	-6.305827	0.472768
1	-1.332361	-4.159976	-0.400839
1	1.269671	-5.375492	-0.805953
1	-0.009141	-5.561207	1.973857
1	-1.645942	-3.889692	1.318198
1	0.390975	-0.265091	2.536710
1	0.372280	-1.375263	2.627298

Full Structure 8 - THF

B3LYP/GBS(1) = -2088.356584 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2088.830506 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2087.707057 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -2083.818686 a.u.
Enthalpy Correction = 0.744873
Gibbs Free Energy Correction = 0.628616

Atomic No	x-coord	y-coord	z-coord
1	-5.434358	4.317910	-1.732355
1	-6.093569	3.159614	-0.568553
6	-5.287090	3.882044	-0.735677
1	-5.421412	4.695678	-0.009845
1	-2.817571	4.921964	-1.350746
6	-2.752165	3.915101	-0.941155
6	-3.930339	3.230686	-0.605115
1	-3.263507	-0.088730	-2.562139
1	-3.576311	-1.781576	-2.987366
1	-5.315397	-0.322848	-0.963489
1	-0.621800	3.916043	-1.058792
6	-1.497116	3.347738	-0.768107
6	-3.783855	1.912676	-0.167609
1	-4.679236	1.346365	0.071073
6	-3.027410	-1.125699	-2.299299
1	-5.455104	-2.051127	-1.276645
1	2.800423	0.240365	-4.013361
6	-4.947524	-1.304403	-0.652104
1	-1.953599	-1.274060	-2.454155

1	2.163866	1.370034	-2.802081
1	1.300947	-0.139111	-3.136576
6	2.295546	0.310396	-3.041250
6	-2.531322	1.297955	-0.032190
6	-1.337339	2.040364	-0.242249
1	-5.262467	-1.477007	0.382444
6	-3.427491	-1.431478	-0.845838
1	0.127191	3.981766	1.000241
1	4.813205	5.251329	-0.166308
1	-3.162253	-2.475387	-0.642717
1	2.193845	5.244855	1.237085
6	1.060394	3.511003	0.714892
7	-0.108103	1.427024	0.006789
6	2.242421	4.225639	0.856783
15	-2.290944	-0.479711	0.330524
6	1.049516	2.180804	0.224906
1	3.864550	-1.930515	-3.330696
6	3.120419	-0.418396	-1.968296
1	-4.075936	-0.321343	1.976133
1	4.095003	0.082266	-1.882651
6	3.489170	3.673233	0.525941
6	4.761117	4.483129	0.617545
1	2.401016	-2.416766	-2.451597
6	2.319883	1.576337	0.019144
1	4.841749	5.004703	1.579800
6	3.352730	-1.884667	-2.360777
6	3.493874	2.334749	0.127706
77	0.023131	-0.690772	0.000550
6	-3.045278	-0.696102	2.044344
1	5.647226	3.847965	0.510051
1	4.448057	1.867658	-0.100446
1	-2.296322	1.227173	2.778489
15	2.289970	-0.225830	-0.290471
1	-3.646145	-2.803390	1.809811
1	3.967745	-2.423356	-1.632539
6	-2.283477	0.170041	3.060156
6	-3.081035	-2.162545	2.496450
1	-2.743380	0.075678	4.052326
1	-3.555701	-2.240494	3.482771
1	-1.237011	-0.145534	3.133970
1	-2.064981	-2.563188	2.585743
1	5.328955	-0.927454	-0.193999
1	5.204787	0.286802	1.093775
6	3.451822	-1.024327	0.962005
6	4.955704	-0.742674	0.818863
1	3.281013	-2.089533	0.774002
1	3.079933	0.346693	2.626976
1	1.904511	-0.974976	2.502658
6	2.962131	-0.716147	2.386931
1	5.513636	-1.401107	1.497580
1	3.545516	-1.292572	3.116735
6	1.334490	-4.647651	-0.264068
6	-0.058714	-4.997678	0.247759
6	-0.832328	-3.722051	-0.115506
6	0.195563	-2.589204	-0.063656
8	1.418765	-3.210394	-0.137811
1	2.157602	-5.078538	0.311829
1	-0.463172	-5.905527	-0.209378
1	-1.220885	-3.781502	-1.143401
1	1.466903	-4.911310	-1.321890
1	-0.041596	-5.139790	1.334405

1	-1.679579	-3.534827	0.542475

Full Structure 9 - THF

B3LYP/GBS(1) = -2089.520045 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2090.004939 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2088.876561 a.u.
Enthalpy Correction = 0.763208
Gibbs Free Energy Correction = 0.649148

Atomic No	x-coord	y-coord	z-coord
1	-5.711761	3.185556	-2.600849
1	-6.239284	2.494948	-1.059637
6	-5.478901	3.128090	-1.529696
1	-5.599652	4.141388	-1.123228
1	-3.105425	3.961487	-2.633041
6	-2.965692	3.150868	-1.919603
6	-4.088463	2.589629	-1.287376
1	-4.563960	-0.898855	-1.383199
1	-4.557226	-2.669429	-1.359717
1	-5.419868	-0.791098	1.084313
1	-0.847635	3.141872	-2.203877
6	-1.679666	2.695252	-1.671149
6	-3.855874	1.501334	-0.445727
1	-4.710616	1.027250	0.031007
6	-3.962883	-1.775988	-1.129458
1	-5.547837	-2.539919	0.890772
1	4.439547	-2.831377	-1.895396
6	-4.876352	-1.733535	1.212570
1	-3.094415	-1.774168	-1.791554
1	3.188052	-3.142952	-0.680038
1	4.747085	-2.458489	-0.201306
6	3.974976	-2.445201	-0.978646
6	-2.569949	0.993799	-0.202674
6	-1.423676	1.637318	-0.757462
1	-4.689247	-1.872975	2.280273
6	-3.590828	-1.781485	0.366845
1	-0.081141	3.914158	-0.348884
1	4.793895	5.012237	-0.648116
1	-3.091288	-2.734502	0.590532
1	1.889274	5.285154	-0.058360
6	0.878593	3.420410	-0.266920
7	-0.156472	1.171405	-0.444170
6	2.005530	4.202479	-0.081531
15	-2.236787	-0.509252	0.790823
6	0.939342	1.996695	-0.295131
1	5.158138	-0.551706	-2.464698
6	3.453704	-1.018633	-1.222743
1	-3.677249	0.116056	2.638159
1	2.756273	-1.035698	-2.066405
6	3.281207	3.643078	0.103271

6	4.506326	4.507606	0.284863
1	5.361019	-0.011645	-0.796467
6	2.225359	1.424579	-0.049079
1	4.342218	5.293704	1.033178
6	4.630563	-0.109038	-1.609458
6	3.347435	2.252064	0.132207
77	0.025595	-0.896954	0.289329
6	-2.592851	-0.042767	2.581037
1	5.367677	3.914486	0.611792
1	4.310769	1.791341	0.335442
1	-2.226288	2.102877	2.336325
15	2.322008	-0.392441	0.167003
1	-2.700583	-2.126456	3.300950
1	4.302707	0.891162	-1.898705
6	-1.908719	1.274208	2.975836
6	-2.197714	-1.181436	3.535823
1	-2.169572	1.523618	4.012268
1	-2.459482	-0.913376	4.567238
1	-0.819259	1.194727	2.910251
1	-1.119338	-1.362464	3.489628
1	3.148550	1.367649	2.568484
1	1.915493	0.244956	3.158790
6	3.313158	-0.675145	1.759022
6	2.967545	0.333171	2.867282
1	4.369240	-0.537475	1.484326
1	2.070190	-2.270794	2.554882
1	3.415010	-2.878187	1.588075
6	3.120657	-2.103672	2.299524
1	3.578640	0.119547	3.753633
1	3.725111	-2.237200	3.206000
6	1.128964	-2.939325	-3.034398
6	0.484680	-3.594650	-1.794274
6	-0.536867	-2.543588	-1.383980
6	-0.320214	-1.423116	-2.148252
8	0.746640	-1.537613	-3.005792
1	2.218364	-2.990094	-3.052369
1	-0.002288	-4.541932	-2.052144
1	-1.478394	-2.836034	-0.953131
1	-0.951915	-0.566272	-2.336104
1	0.170080	-2.316529	1.054731
1	0.268450	-0.277786	1.736970
1	0.742504	-3.363343	-3.969727
1	1.202122	-3.799521	-0.995570

Full Structure 10 - THF

B3LYP/GBS(1) = -2089.519231 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2090.007171 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2088.881627 a.u.
Enthalpy Correction = 0.762676
Gibbs Free Energy Correction = 0.650146

Atomic No	x-coord	y-coord	z-coord
1	-5.474695	3.770499	-2.372580

1	-6.191710	2.721277	-1.142131
6	-5.403168	3.460155	-1.321899
1	-5.636475	4.343776	-0.712703
1	-2.942479	4.614116	-1.709289
6	-2.866953	3.633310	-1.242477
6	-4.039387	2.898189	-0.996212
1	-3.977228	-0.624886	-2.201952
1	-3.941233	-2.377708	-2.469624
1	-5.460715	-0.963693	-0.048352
1	-0.736801	3.744688	-1.159224
6	-1.608752	3.146006	-0.923887
6	-3.876782	1.621294	-0.459327
1	-4.763167	1.017656	-0.282351
6	-3.445130	-1.547905	-1.951152
1	-5.440610	-2.674506	-0.474686
1	2.590458	0.729350	-4.008429
6	-4.907491	-1.898300	0.088770
1	-2.427071	-1.451542	-2.339591
1	1.928461	1.669132	-2.657846
1	1.137321	0.164860	-3.153760
6	2.107666	0.654478	-3.025685
6	-2.614079	1.091216	-0.157518
6	-1.437047	1.868578	-0.329246
1	-4.958568	-2.169923	1.146866
6	-3.462884	-1.798553	-0.432766
1	-0.151981	3.866611	1.026323
1	4.505960	5.393159	0.171131
1	-2.984705	-2.771288	-0.246316
1	1.844749	5.221891	1.380920
6	0.818141	3.446677	0.787000
7	-0.209321	1.331327	0.023256
6	1.955994	4.210623	0.992991
15	-2.314133	-0.591230	0.459816
6	0.896666	2.119460	0.289602
1	3.733792	-1.436180	-3.656693
6	3.007754	-0.147858	-2.073875
1	-4.001743	-0.391461	2.182541
1	3.951778	0.401926	-1.957490
6	3.242249	3.713730	0.722760
6	4.471615	4.573307	0.901537
1	2.392998	-2.135851	-2.727261
6	2.195580	1.577860	0.117603
1	4.504584	5.033307	1.897636
6	3.305770	-1.538625	-2.651378
6	3.327340	2.387812	0.298124
77	-0.011854	-0.789290	0.035027
6	-2.918984	-0.566120	2.244474
1	5.389058	3.987632	0.777772
1	4.312191	1.974989	0.103334
1	-2.547141	1.567119	2.579144
15	2.270022	-0.191782	-0.337843
1	-3.094839	-2.759171	2.444502
1	4.028886	-2.098505	-2.047508
6	-2.290186	0.600557	3.021902
6	-2.666403	-1.897043	2.969417
1	-2.657884	0.592297	4.055924
1	-3.113549	-1.867721	3.970822
1	-1.199104	0.512843	3.043207
1	-1.591231	-2.065704	3.090202
1	5.312754	-0.889466	-0.674193
1	5.383097	0.344937	0.594719

6	3.620885	-0.961400	0.752543
6	5.089073	-0.685678	0.376490
1	3.458088	-2.035681	0.618269
1	3.566872	0.421863	2.442365
1	2.348469	-0.854665	2.534009
6	3.377627	-0.636709	2.236245
1	5.736501	-1.334514	0.980449
1	4.057896	-1.229849	2.860895
6	1.847327	-4.011569	-0.448450
6	1.239126	-3.708786	0.943359
6	-0.025235	-2.927851	0.606405
6	-0.129446	-2.885668	-0.798849
8	0.945465	-3.469332	-1.438271
1	2.830016	-3.557182	-0.598215
1	0.967217	-4.637606	1.460689
1	-0.889896	-3.092919	1.234826
1	-1.032134	-2.938916	-1.389057
1	-0.336916	-0.621632	-1.597180
1	0.312793	-0.652402	1.674682
1	1.942806	-5.085744	-0.644053
1	1.925751	-3.166500	1.596936

Full Structure 12 - THF

B3LYP/GBS(1) = -2088.336985 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2088.814325 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2087.701341 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -2083.806842 a.u.
Enthalpy Correction = 0.745078
Gibbs Free Energy Correction = 0.631825

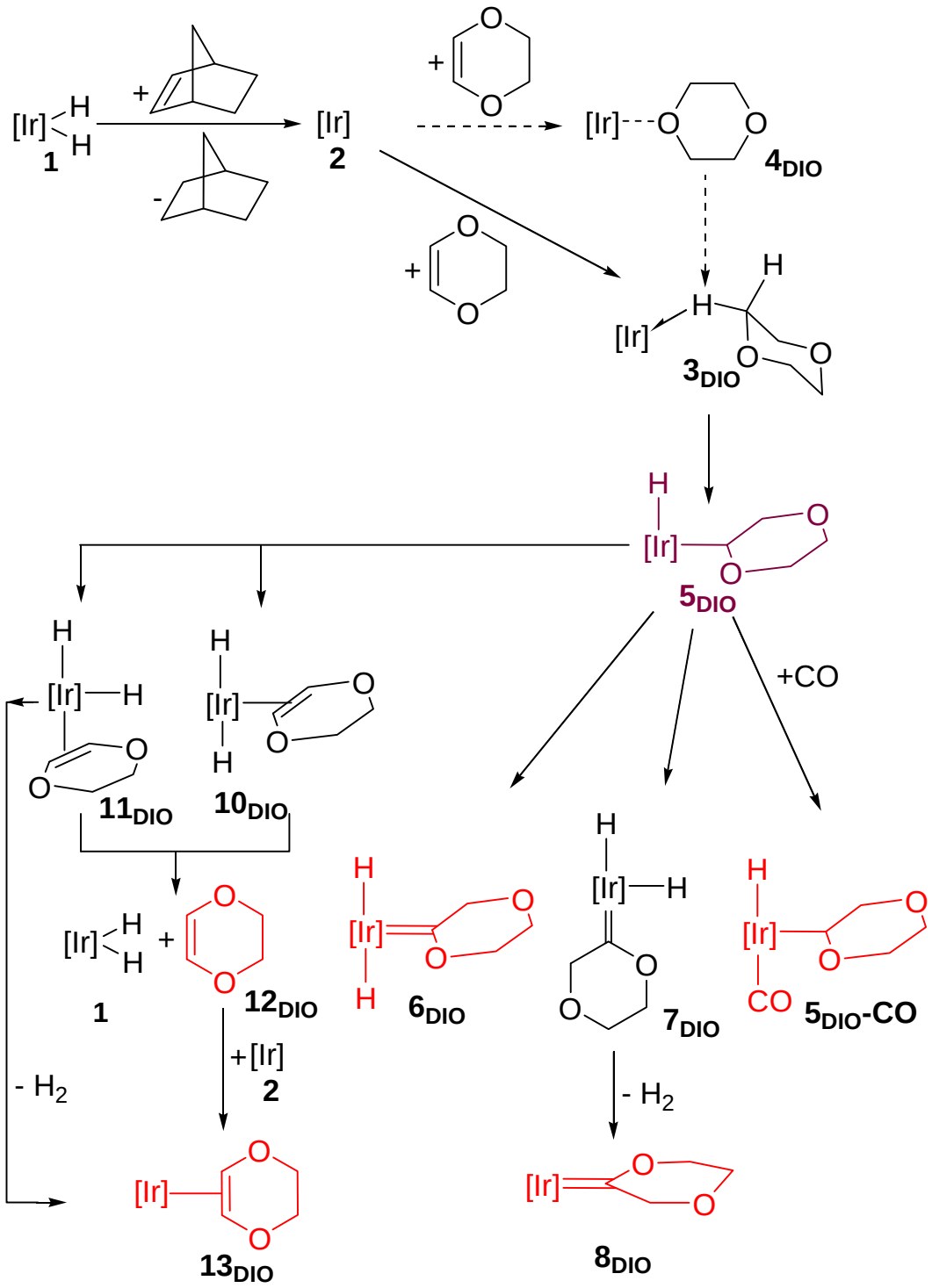
Atomic No	x-coord	y-coord	z-coord
1	-5.543622	3.889593	-2.121357
1	-6.227056	2.752628	-0.950510
6	-5.442760	3.502822	-1.099248
1	-5.656694	4.338903	-0.419634
1	-2.988910	4.622487	-1.617648
6	-2.903942	3.638727	-1.158877
6	-4.070773	2.919375	-0.855678
1	-3.823748	-0.457910	-2.312781
1	-3.769564	-2.185424	-2.711771
1	-5.437237	-0.955769	-0.326513
1	-0.770160	3.725773	-1.169453
6	-1.636682	3.133824	-0.899634
6	-3.897324	1.634682	-0.336910
1	-4.781001	1.039471	-0.121258
6	-3.307605	-1.399728	-2.101124
1	-5.378832	-2.651849	-0.802961
1	2.686032	0.423153	-4.008338
6	-4.887398	-1.891262	-0.182743
1	-2.267338	-1.281862	-2.420255
1	1.818760	1.350666	-2.769448
1	1.298439	-0.295805	-3.161764

6	2.173414	0.351393	-3.040562
6	-2.628833	1.088472	-0.101329
6	-1.455053	1.857089	-0.313452
1	-5.003523	-2.196258	0.861277
6	-3.415348	-1.763748	-0.608821
1	-0.165591	3.847290	1.013074
1	4.446092	5.436058	-0.020940
1	-2.944351	-2.747253	-0.468171
1	1.815482	5.237394	1.314608
6	0.804586	3.441187	0.751270
7	-0.208253	1.299526	-0.004312
6	1.935103	4.227665	0.925178
15	-2.304113	-0.628630	0.411989
6	0.895123	2.119617	0.249551
1	4.180617	-1.492669	-3.384760
6	3.131060	-0.223093	-1.983371
1	-4.028975	-0.468145	2.105464
1	3.977658	0.468739	-1.873607
6	3.219802	3.757596	0.611826
6	4.436206	4.644381	0.740664
1	2.845955	-2.305587	-2.543386
6	2.197633	1.597091	0.056386
1	4.473309	5.142493	1.717905
6	3.665410	-1.593344	-2.420794
6	3.318176	2.428954	0.192523
77	-0.002861	-0.779721	0.019878
6	-2.961652	-0.719758	2.176642
1	5.362373	4.070699	0.626271
1	4.304236	2.033391	-0.032043
1	-2.422275	1.349122	2.662219
15	2.273871	-0.199313	-0.302495
1	-3.263651	-2.909412	2.196653
1	4.386573	-2.010172	-1.708928
6	-2.273795	0.338663	3.053831
6	-2.822023	-2.114242	2.807707
1	-2.685645	0.303452	4.070518
1	-3.324593	-2.131629	3.782954
1	-1.195610	0.154519	3.114364
1	-1.768362	-2.359645	2.974780
1	5.373621	-0.587639	-0.202608
1	5.144655	0.533243	1.152971
6	3.509319	-0.907536	0.940705
6	4.985716	-0.494967	0.816561
1	3.453689	-1.984785	0.747004
1	3.043691	0.411714	2.616139
1	1.952255	-0.974623	2.481938
6	2.993217	-0.654272	2.368530
1	5.596159	-1.141754	1.460151
1	3.610072	-1.198696	3.095124
6	1.874468	-3.979072	-0.452280
6	1.195466	-3.717194	0.914983
6	-0.036140	-2.897966	0.542555
6	-0.036838	-2.738929	-0.867986
8	1.092394	-3.310150	-1.461934
1	2.899263	-3.598934	-0.501419
1	0.889125	-4.661337	1.383770
1	-0.945446	-3.134954	1.083831
1	-0.893013	-2.811366	-1.533514
1	1.906175	-5.046487	-0.705510
1	1.862331	-3.217200	1.623567

4. Dioxane (DIO)

4.1. Dioxane (DIO) relative energy diagrams.

Scheme S4



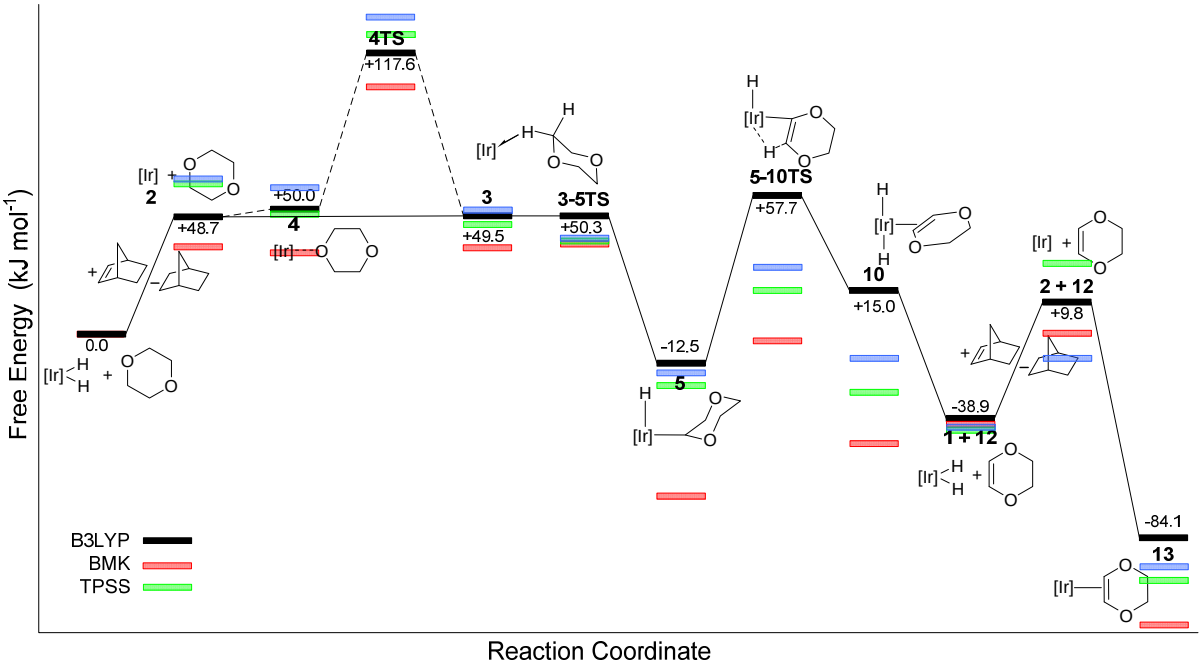


Figure S21. Relative energy surface for the formation of vinyl ether adduct **13**$_{DIO}$. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

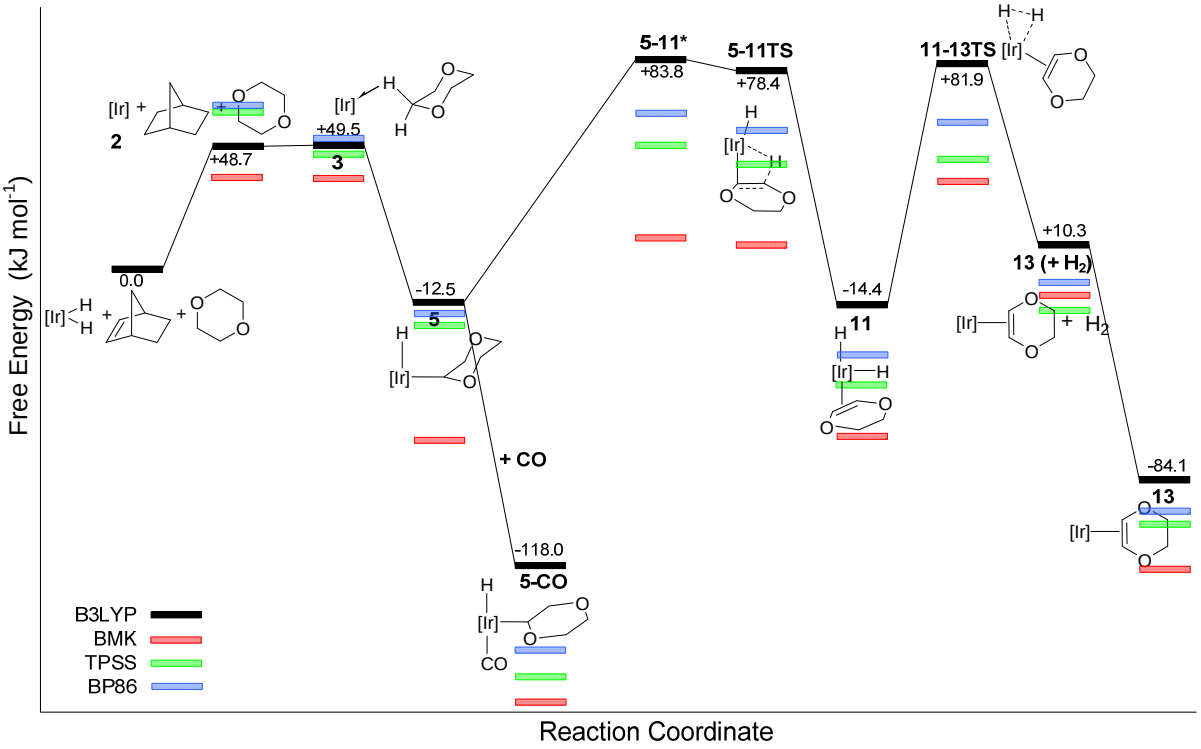


Figure S22. Relative energy surface for the formation of vinyl ether adduct **13**$_{DIO}$ and CO trapped intermediate **5-CO**$_{DIO}$. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

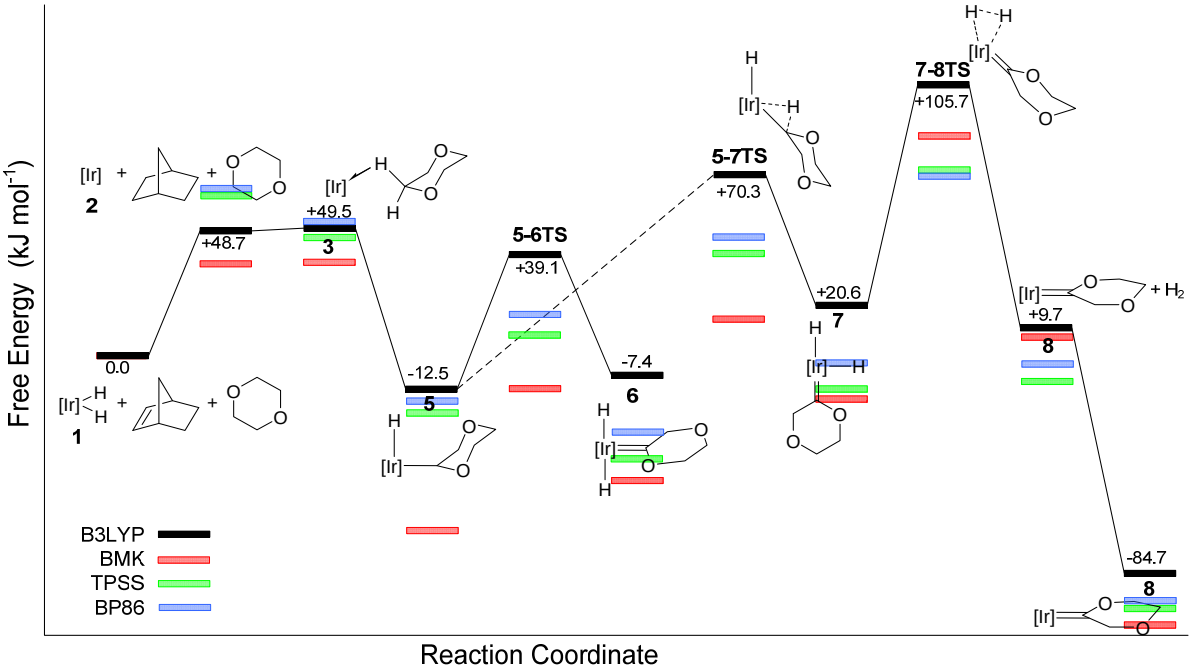


Figure S23. Relative energy surface for the formation of carbene **8**$_{DIO}$. Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

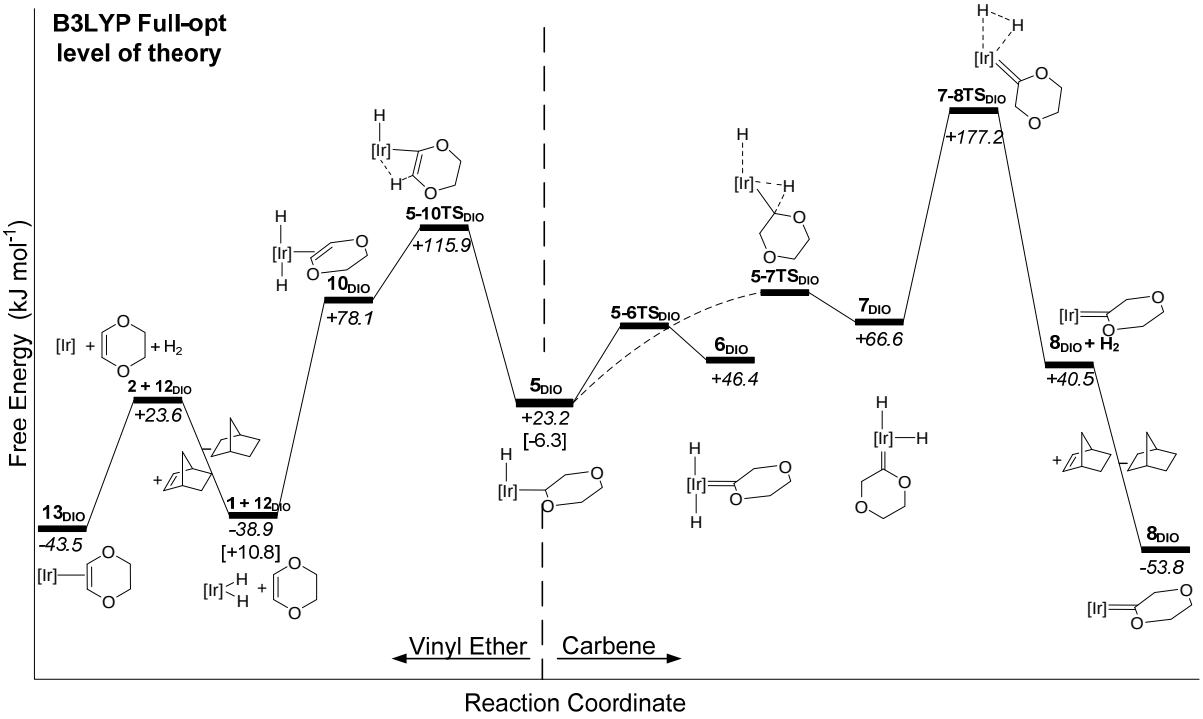


Figure S24. Relative energy surface for the formation of carbene **8**$_{DIO}$ to the right and vinyle ether adduct to the left. Values are B3LYP Gibbs corrected Full-opt energies. Drawn to scale with all values in kJ mol^{-1}.

4.2. Coordinates of DIO structures at the Model-opt level of theory

Structure 1,4-dioxane (DIO)

B3LYP/GBS(1) = -307.653141 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -307.759548 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -307.571387 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -307.801846 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -307.7545667 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -307.5578676 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -306.958422 a.u.
Enthalpy Correction = 0.12936
Gibbs Free Energy Correction = 0.094866

Atomic No	x-coord	y-coord	z-coord
6	1.171198	-0.737604	0.194483
6	1.171193	0.737613	-0.194483
8	-0.000008	1.383140	0.293326
6	-1.171228	0.737579	-0.194565
6	-1.171222	-0.737587	0.194565
8	0.000002	-1.383140	-0.293326
1	2.025443	-1.262968	-0.245031
1	2.025433	1.262982	0.245031
1	-2.025436	1.263075	0.244831
1	-1.224310	-0.828967	1.292318
1	-2.025427	-1.263089	-0.244831
1	-1.224316	0.828958	-1.292318
1	1.224508	0.829073	-1.292237
1	1.224514	-0.829064	1.292237

Structure 3 - DIO

B3LYP/GBS(1) = -1464.330349 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.644212 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.412520 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.721050 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.767208 a.u.
Enthalpy Correction = 0.374411
Gibbs Free Energy Correction = 0.298531

Atomic No	x-coord	y-coord	z-coord		
1	7	0	-2.393328	0.475637	-0.168516
2	6	0	-2.806333	1.781701	-0.232033
3	6	0	-1.946568	2.832641	-0.156112
4	1	0	-3.880865	1.935505	-0.350967
5	1	0	-2.301485	3.856911	-0.211642
6	6	0	-3.311535	-0.534881	-0.278473
7	6	0	-2.965940	-1.849733	-0.242437
8	1	0	-4.351278	-0.224363	-0.400016
9	1	0	-3.711036	-2.633990	-0.331131
10	15	0	-0.226736	2.360207	0.019799
11	15	0	-1.210135	-2.139516	-0.036182
12	6	0	0.450562	3.258039	1.492601

13	1	0	1.510928	3.009679	1.607805
14	1	0	0.344386	4.343760	1.382592
15	1	0	-0.088033	2.934655	2.387614
16	6	0	0.698839	3.192068	-1.354496
17	1	0	0.527904	4.275039	-1.345988
18	1	0	1.771660	3.003462	-1.245398
19	1	0	0.362152	2.782674	-2.310570
20	6	0	-1.046283	-3.296642	1.407661
21	1	0	-1.656219	-4.196007	1.262247
22	1	0	-0.002394	-3.602980	1.540571
23	1	0	-1.377796	-2.783278	2.314284
24	6	0	-0.676491	-3.241064	-1.430643
25	1	0	0.383150	-3.499845	-1.327421
26	1	0	-1.265935	-4.165230	-1.456046
27	1	0	-0.810292	-2.704087	-2.373436
28	77	0	-0.423823	0.046978	0.060354
29	6	0	4.447483	-0.729643	-0.607519
30	6	0	3.687918	0.591869	-0.649156
31	6	0	2.017217	-0.326476	0.725316
32	6	0	2.776065	-1.651622	0.745493
33	1	0	5.177850	-0.711376	0.218240
34	1	0	3.027923	0.617926	-1.530017
35	1	0	1.476506	-0.161118	1.659626
36	1	0	2.085136	-2.496368	0.798236
37	8	0	3.545590	-1.817865	-0.437145
38	8	0	2.908485	0.758623	0.538490
39	1	0	1.347660	-0.388265	-0.236169
40	1	0	3.433260	-1.670100	1.631315
41	1	0	4.980776	-0.906291	-1.546796
42	1	0	4.374576	1.442995	-0.690776

Structure 4 (oxygen bound ether)

B3LYP/GBS(1) = -1464.334148a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.643605 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.414409 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.719933 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.762722 a.u.
Enthalpy Correction = 0.375848
Gibbs Free Energy Correction = 0.298086

Atomic	No	x-coord	y-coord	z-coord
7		2.413995	0.252288	-0.016146
6		2.970562	1.503066	-0.018722
6		2.222189	2.640703	-0.005659
1		4.061926	1.543461	-0.032087
1		2.685726	3.622392	-0.007683
6		3.228004	-0.846623	-0.034051
6		2.740481	-2.117956	-0.036673
1		4.302420	-0.651261	-0.047366
1		3.402003	-2.978677	-0.051443
15		0.455261	2.348944	0.014734
15		0.952068	-2.216331	-0.013640
6		-0.264529	3.313505	-1.401047
1		-1.357181	3.229004	-1.396878
1		0.004989	4.374669	-1.338986
1		0.115317	2.902623	-2.340353

6	-0.229563	3.311305	1.449805
1	0.054062	4.369053	1.391630
1	-1.323443	3.244119	1.462661
1	0.159052	2.887893	2.379943
6	0.482928	-3.319591	-1.437705
1	1.016550	-4.276459	-1.390350
1	-0.594636	-3.522183	-1.429872
1	0.737246	-2.817033	-2.374962
6	0.520605	-3.335087	1.409716
1	-0.555100	-3.547257	1.421062
1	1.060243	-4.287473	1.343164
1	0.790084	-2.838465	2.345850
77	0.394002	0.037370	0.008223
6	-3.883751	-0.047567	-1.236023
6	-2.481833	-0.659350	-1.117724
6	-2.475140	-0.390240	1.270623
6	-3.964418	-0.679389	1.036634
1	-4.520540	-0.707834	-1.847391
1	-1.861740	-0.415521	-1.980942
1	-1.972137	-1.240276	1.747770
1	-4.528219	-0.481898	1.953060
8	-4.480205	0.183018	0.040157
8	-1.821448	-0.085011	0.017341
1	-2.332992	0.496353	1.891780
1	-4.128652	-1.735774	0.769656
1	-3.832645	0.929778	-1.726195
1	-2.508415	-1.752631	-1.013682

Structure 3-5TS - DIO

B3LYP/GBS(1) = -1464.326086 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.642164 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.410869 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.722592 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.770521 a.u.
Enthalpy Correction = 0.370505
Gibbs Free Energy Correction = 0.296786
Imaginary Freq = -653.4 i

Atomic No	x-coord	y-coord	z-coord
7	-2.316556	0.623687	-0.112637
6	-2.647660	1.952630	-0.186531
6	-1.721230	2.947068	-0.145720
1	-3.712175	2.178989	-0.285796
1	-2.012057	3.991370	-0.203207
6	-3.288306	-0.333510	-0.243973
6	-3.011079	-1.664448	-0.250482
1	-4.313534	0.029340	-0.350606
1	-3.797485	-2.406368	-0.347906
15	-0.023618	2.378878	-0.006438
15	-1.271292	-2.064081	-0.057608
6	0.725514	3.251852	1.444765
1	1.770099	2.941494	1.546238
1	0.679177	4.340473	1.324096
1	0.182194	2.970086	2.351107
6	0.912604	3.140305	-1.410863

1	0.794762	4.230125	-1.416866
1	1.976083	2.899528	-1.317491
1	0.537815	2.732553	-2.353274
6	-1.205611	-3.268942	1.354306
1	-1.890394	-4.107059	1.179898
1	-0.194312	-3.669775	1.482168
1	-1.498589	-2.756167	2.274588
6	-0.783706	-3.143568	-1.481915
1	0.269211	-3.430670	-1.388540
1	-1.401145	-4.048033	-1.531484
1	-0.903728	-2.574068	-2.407297
77	-0.341434	0.069202	0.068628
6	4.083107	-1.097216	-0.653686
6	3.493032	0.309326	-0.683621
6	1.796442	-0.360836	0.826710
6	2.415653	-1.757454	0.843347
1	4.868595	-1.155580	0.118041
1	2.792805	0.400083	-1.529067
1	1.415588	-0.108303	1.819620
1	1.653939	-2.524131	0.994003
8	3.067335	-2.057199	-0.384822
8	2.808476	0.599709	0.534086
1	1.151592	-0.434560	-0.423936
1	3.144067	-1.811878	1.671400
1	4.519950	-1.360184	-1.622299
1	4.278485	1.065086	-0.786756

Structure 4-5TS - DIO

B3LYP/GBS(1) = -1464.306958 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.615675 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.385242 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.688495 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.733441 a.u.
Enthalpy Correction = 0.374546
Gibbs Free Energy Correction = 0.295935
Imaginary Freq = -75.2 i

Atomic No	x-coord	y-coord	z-coord
7	-0.891850	-1.110287	3.833037
6	-1.374381	0.082456	4.314968
6	-1.082606	1.283878	3.750769
1	-2.018668	0.004670	5.192374
1	-1.480299	2.206868	4.160802
6	-1.247892	-2.290907	4.433007
6	-0.828640	-3.503869	3.983831
1	-1.898701	-2.197393	5.303898
1	-1.126652	-4.421956	4.480204
15	-0.009023	1.176855	2.318174
15	0.223128	-3.421082	2.535530
6	1.410543	2.330763	2.613713
1	2.100400	2.300405	1.763868
1	1.060363	3.359981	2.757023
1	1.946716	2.009985	3.511396
6	-0.872277	2.022060	0.913107
1	-1.107991	3.065332	1.154426

1	-0.229844	1.994443	0.026939
1	-1.797065	1.484209	0.688542
6	1.756267	-4.387106	2.941227
1	1.510552	-5.408109	3.256301
1	2.413601	-4.439726	2.065742
1	2.290988	-3.881396	3.749780
6	-0.547072	-4.515449	1.249866
1	0.092408	-4.560899	0.361241
1	-0.697478	-5.533199	1.629063
1	-1.512620	-4.092518	0.960182
77	0.292285	-1.121080	2.225219
6	3.994596	0.017418	0.935276
6	2.942264	-0.846244	0.203773
6	2.622499	0.755559	-1.499052
6	4.052445	1.176812	-1.099288
1	4.964904	-0.506179	0.961074
1	2.376925	-1.442093	0.941454
1	2.638462	0.191687	-2.446548
1	4.302707	2.155688	-1.518460
8	4.136570	1.291411	0.310159
8	2.008220	-0.016741	-0.468782
1	1.979295	1.630602	-1.630756
1	4.797783	0.453694	-1.469887
1	3.677953	0.219447	1.961045
1	3.411290	-1.549417	-0.503947

Structure 5 - DIO

B3LYP/GBS(1) = -1464.350076 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.665527 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.450213 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.745118 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.790691 a.u.
Enthalpy Correction = 0.371051
Gibbs Free Energy Correction = 0.296237

Atomic No	x-coord	y-coord	z-coord
7	2.238996	1.078673	-0.047966
6	3.376370	0.331940	-0.060927
6	3.360578	-1.032404	0.001723
1	4.326749	0.870550	-0.128855
1	4.283618	-1.604333	-0.011715
6	2.262647	2.434083	-0.205592
6	1.126650	3.187647	-0.259278
1	3.246163	2.906567	-0.290514
1	1.179104	4.266198	-0.374285
15	1.742052	-1.806431	0.066605
15	-0.424140	2.294314	-0.081804
6	1.717575	-2.906727	1.558069
1	0.767945	-3.450778	1.605331
1	2.541286	-3.629270	1.531744
1	1.815154	-2.295491	2.460193
6	1.696161	-3.042999	-1.309481

1	2.564768	-3.708963	-1.255226
1	0.784208	-3.645937	-1.257401
1	1.712747	-2.513536	-2.265769
6	-1.295833	3.009229	1.383450
1	-1.480794	4.080982	1.247992
1	-2.241876	2.479058	1.516107
1	-0.678237	2.868536	2.275725
6	-1.540143	2.754086	-1.474899
1	-2.469056	2.188260	-1.362053
1	-1.754725	3.828521	-1.477317
1	-1.067033	2.479724	-2.421510
77	0.330385	0.084212	0.055379
6	-3.851761	-0.446662	0.753298
6	-4.237108	-1.470257	-0.308777
6	-1.960901	-1.848502	-0.731097
6	-1.532530	-0.825954	0.316342
1	-3.791550	-0.946094	1.735546
1	-4.390252	-0.952929	-1.272725
1	0.221084	-0.016748	-1.488680
8	-2.605309	0.157989	0.433271
8	-3.227143	-2.455798	-0.433609
1	-2.015831	-1.368695	-1.722073
1	-1.499670	-1.358659	1.292486
1	-4.594902	0.358169	0.814325
1	-5.163649	-1.991842	-0.041743
1	-1.247157	-2.674955	-0.784282

Structure 5-6TS - DIO

B3LYP/GBS(1) = -1464.321675 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.641792 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.425083 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.729092 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.774249 a.u.
Enthalpy Correction = 0.365747
Gibbs Free Energy Correction = 0.292120
Imaginary Freq = -845.6 i

Atomic No	x-coord	y-coord	z-coord
7	-2.103275	1.060569	-0.548453
6	-3.231271	0.321835	-0.694482
6	-3.263762	-1.018693	-0.450310
1	-4.134259	0.851063	-1.013517
1	-4.174686	-1.594614	-0.583958
6	-2.126471	2.413358	-0.665719
6	-1.039793	3.193495	-0.402222
1	-3.072058	2.865961	-0.979132
1	-1.080730	4.272235	-0.519416
15	-1.733671	-1.769394	0.099915
15	0.443293	2.332256	0.114575
6	-1.517795	-3.240312	-1.015605
1	-0.755679	-3.930202	-0.638405
1	-2.464933	-3.786892	-1.091179

1	-1.227229	-2.898822	-2.012971
6	-2.089478	-2.610804	1.711860
1	-2.943940	-3.291376	1.620746
1	-1.215828	-3.182347	2.044233
1	-2.312559	-1.847325	2.460964
6	1.778212	2.889217	-1.040002
1	1.829402	3.983969	-1.065396
1	2.743580	2.490098	-0.718922
1	1.554934	2.519009	-2.044141
6	1.009672	3.066643	1.712793
1	1.945018	2.588567	2.021129
1	1.171908	4.146515	1.617823
1	0.250646	2.878889	2.475909
77	-0.278142	0.101943	0.122462
6	3.834491	-0.363271	-0.409368
6	4.095946	-1.829688	-0.136551
6	1.804584	-2.194347	0.096797
6	1.486779	-0.704940	0.109543
1	3.755174	-0.189321	-1.490125
1	4.262731	-1.996743	0.941237
1	-0.978726	0.452891	1.549586
8	2.602603	0.074076	0.208185
8	2.987560	-2.581177	-0.594058
1	1.882944	-2.494446	1.158640
1	4.614367	0.281774	0.004976
1	4.976744	-2.177882	-0.685607
1	0.992345	-2.748652	-0.362163
1	0.708387	-0.387003	-1.311491

Structure 5-7TS - DIO

B3LYP/GBS(1) = -1464.309276 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.632051 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.417331 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.719802 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.764768 a.u.
Enthalpy Correction = 0.366864
Gibbs Free Energy Correction = 0.294263
Imaginary Freq = -510.2 i

Atomic No	x-coord	y-coord	z-coord
7	1.877335	1.161286	-0.711975
6	1.781324	2.506812	-0.920288
6	0.679720	3.227656	-0.584574
1	2.651624	2.984774	-1.375006
1	0.621716	4.293612	-0.781669
6	3.061398	0.522122	-0.927758
6	3.266774	-0.779400	-0.594594
1	3.853475	1.118458	-1.385599
1	4.214521	-1.270257	-0.792858
15	-0.656928	2.294873	0.154675

15	1.877848	-1.617181	0.159177
6	-2.167227	2.776665	-0.799021
1	-3.070125	2.417946	-0.299966
1	-2.208606	3.869162	-0.884325
1	-2.122891	2.333561	-1.796009
6	-1.030334	3.037614	1.807878
1	-1.280633	4.100783	1.715801
1	-1.874795	2.512146	2.266768
1	-0.155529	2.922341	2.451860
6	1.762540	-3.219800	-0.776170
1	2.763359	-3.658921	-0.861934
1	1.115016	-3.941961	-0.268660
1	1.372108	-3.033469	-1.780153
6	2.412689	-2.239556	1.819034
1	1.600051	-2.809117	2.283385
1	3.296183	-2.882893	1.735228
1	2.643454	-1.381593	2.454467
77	0.289305	0.140604	0.177260
6	-3.902313	-2.186746	-0.309779
6	-3.760900	-0.726474	0.075771
6	-1.388395	-0.826801	-0.378953
6	-1.583935	-2.321150	-0.565531
1	-4.064586	-2.276587	-1.397757
1	-3.687226	-0.635860	1.169747
1	1.111405	0.649676	1.506748
1	-0.733261	-2.876625	-0.181956
8	-2.732534	-2.883132	0.077892
8	-2.585532	-0.143448	-0.516262
1	-1.009106	-0.692975	1.001412
1	-1.658726	-2.498818	-1.653503
1	-4.747480	-2.651426	0.209364
1	-4.605120	-0.125843	-0.277511

Structure 5-10TS - DIO

B3LYP/GBS(1) = -1464.315383 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.637069 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.424006 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.72796 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.771967 a.u.
Enthalpy Correction = 0.366264
Gibbs Free Energy Correction = 0.294493
Imaginary Freq = -756.7 i

Atomic No	x-coord	y-coord	z-coord
7	1.346193	1.781635	-0.576217
6	2.690438	1.682343	-0.726106
6	3.378668	0.530314	-0.475447
1	3.217566	2.583194	-1.053302
1	4.454175	0.474083	-0.612235
6	0.712596	2.980828	-0.681548

6	-0.609429	3.138400	-0.397598
1	1.321155	3.831988	-1.000017
1	-1.094313	4.104368	-0.504183
15	2.402295	-0.836857	0.133458
15	-1.486631	1.671817	0.149527
6	3.092585	-1.344629	1.773295
1	2.539685	-2.207027	2.162308
1	4.153941	-1.607451	1.696188
1	2.972537	-0.512888	2.471294
6	2.845825	-2.312135	-0.901283
1	3.931553	-2.461903	-0.905502
1	2.376771	-3.222222	-0.509712
1	2.509427	-2.149772	-1.929226
6	-2.229954	2.031665	1.802014
1	-2.929836	2.874048	1.754082
1	-2.753152	1.137340	2.154312
1	-1.424937	2.263825	2.502891
6	-3.009985	1.615554	-0.906044
1	-3.748675	0.932688	-0.476244
1	-3.456693	2.614937	-0.963409
1	-2.750856	1.284579	-1.915241
77	0.239525	0.074267	0.096790
6	-3.081209	-2.339500	0.499162
6	-3.099613	-2.058661	-0.993976
6	-0.716725	-1.911538	-0.743813
6	-0.855057	-1.637044	0.682703
1	-2.781724	-3.382853	0.690814
1	-3.498640	-1.057881	-1.184939
1	0.120141	-2.527800	-1.049937
8	-2.189870	-1.433723	1.134902
8	-1.786189	-2.156581	-1.564343
1	-0.319822	-2.318703	1.349226
1	-4.074619	-2.177959	0.929828
1	-3.709708	-2.788277	-1.536867
1	0.564777	0.631455	1.603219
1	-0.120835	-0.563297	-1.490085

Structure 5-11TS - DIO

B3LYP/GBS(1) = -1464.305395 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.629130 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.419357 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.718822 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.762327 a.u.
Enthalpy Correction = 0.366654
Gibbs Free Energy Correction = 0.294434
Imaginary Freq = -306.1 i

Atomic No	x-coord	y-coord	z-coord
7	-1.000389	-1.503419	1.087427
6	-2.288012	-1.401878	1.514863

6	-3.144984	-0.439924	1.069431
1	-2.614240	-2.150155	2.240700
1	-4.165755	-0.382806	1.434109
6	-0.228363	-2.573593	1.440398
6	1.006501	-2.797998	0.918757
1	-0.665659	-3.259415	2.169275
1	1.598025	-3.654572	1.226842
15	-2.474233	0.668433	-0.162430
15	1.562508	-1.604108	-0.297795
6	-2.846395	2.394804	0.405318
1	-2.515449	3.125068	-0.342159
1	-3.923509	2.522708	0.561725
1	-2.328920	2.593796	1.347504
6	-3.536658	0.566092	-1.672213
1	-4.583479	0.793045	-1.438647
1	-3.179051	1.272358	-2.429437
1	-3.461306	-0.445138	-2.078222
6	3.277668	-1.110599	0.173797
1	3.922555	-1.995135	0.230085
1	3.674855	-0.421604	-0.578076
1	3.246474	-0.601043	1.137074
6	1.883590	-2.514799	-1.874860
1	2.257549	-1.816257	-2.631229
1	2.622392	-3.311468	-1.728662
1	0.944205	-2.943107	-2.230824
77	-0.273867	-0.142253	-0.300737
6	2.612231	2.494257	1.360208
6	3.013636	2.650867	-0.122538
6	0.799625	1.883462	-0.573907
6	0.610405	1.471641	0.839075
1	2.037001	3.369190	1.704756
1	3.998680	2.214601	-0.311351
1	-0.868094	-1.144992	-1.483212
8	1.841082	1.315123	1.530429
8	2.131220	1.943381	-1.007606
1	0.360305	0.995967	-1.475107
1	-0.069472	2.108092	1.414535
1	3.503212	2.404546	1.990407
1	3.052206	3.714039	-0.404775
1	0.189965	2.722831	-0.929760

Structure 5-11* - DIO (A very weak but stable agostic minima close to 5-11TS)

B3LYP/GBS(1) = -1464.305523 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.628359 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.4197801 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.717379 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.760434 a.u.
Enthalpy Correction = 0.368755
Gibbs Free Energy Correction = 0.295744

Atomic No	x-coord	y-coord	z-coord
7	-1.023232	-1.504717	1.067579

6	-2.312016	-1.391510	1.491763
6	-3.156330	-0.415839	1.054115
1	-2.646451	-2.143721	2.209113
1	-4.177548	-0.350970	1.415935
6	-0.266307	-2.587495	1.418935
6	0.969194	-2.823931	0.906272
1	-0.719908	-3.270422	2.139911
1	1.547179	-3.690064	1.213045
15	-2.464234	0.696928	-0.160688
15	1.547944	-1.625592	-0.294469
6	-2.812411	2.422004	0.424832
1	-2.465461	3.155401	-0.312202
1	-3.888219	2.565325	0.576608
1	-2.296544	2.601207	1.371751
6	-3.519087	0.627560	-1.677869
1	-4.563384	0.870095	-1.448620
1	-3.145310	1.335172	-2.426061
1	-3.457784	-0.380752	-2.093277
6	3.262373	-1.150987	0.198201
1	3.897517	-2.042409	0.257228
1	3.674825	-0.461326	-0.544656
1	3.224258	-0.644748	1.162920
6	1.874438	-2.526311	-1.876199
1	2.262758	-1.825760	-2.623454
1	2.604240	-3.331212	-1.729694
1	0.934075	-2.942216	-2.243993
77	-0.278049	-0.149790	-0.294661
6	2.620689	2.483624	1.373554
6	3.017986	2.691180	-0.108422
6	0.838663	1.887898	-0.606255
6	0.623927	1.456207	0.816595
1	2.042979	3.345577	1.746554
1	4.029848	2.324315	-0.302067
1	-0.876132	-1.128559	-1.503080
8	1.856235	1.297053	1.508907
8	2.187372	1.938275	-1.001549
1	0.411066	1.068175	-1.452849
1	-0.033192	2.124152	1.385160
1	3.512429	2.377073	2.000025
1	2.986380	3.759318	-0.374675
1	0.263587	2.766173	-0.932440

Structure 5-CO - DIO

B3LYP/GBS(1) = -1577.722219 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1578.080225 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1576.811329 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1578.185690 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1578.213754 a.u.
Enthalpy Correction = 0.383106
Gibbs Free Energy Correction = 0.304924

Atomic No	x-coord	y-coord	z-coord

7	2.125109	1.248623	-0.327046
6	3.305933	0.598028	-0.477235
6	3.419102	-0.761188	-0.395184
1	4.188763	1.211718	-0.680398
1	4.382315	-1.249084	-0.510176
6	1.989712	2.580200	-0.565332
6	0.780488	3.212867	-0.566469
1	2.906340	3.141831	-0.768937
1	0.712313	4.281399	-0.747470
15	1.903897	-1.683041	-0.142881
15	-0.669033	2.192644	-0.283582
6	2.156617	-2.804837	1.305296
1	1.262235	-3.417265	1.463112
1	3.014735	-3.466954	1.143670
1	2.333969	-2.205273	2.202170
6	1.738034	-2.895665	-1.525182
1	2.624447	-3.537254	-1.586492
1	0.855768	-3.525414	-1.369452
1	1.620469	-2.349247	-2.463822
6	-1.628722	2.932084	1.106954
1	-1.948673	3.952259	0.866649
1	-2.502025	2.302766	1.298348
1	-1.006172	2.955008	2.005491
6	-1.821136	2.415953	-1.704737
1	-2.720977	1.818727	-1.530186
1	-2.102303	3.469217	-1.817172
1	-1.334729	2.068874	-2.619356
77	0.335635	0.080551	0.036933
6	-3.684862	-1.059057	0.934221
6	-4.189615	-1.545166	-0.420632
6	-1.985961	-1.532615	-1.228698
6	-1.450145	-1.063948	0.119256
1	-3.494859	-1.927387	1.586686
1	-4.483115	-0.674539	-1.034502
8	-2.492078	-0.296303	0.778533
8	-3.190057	-2.299965	-1.082967
1	-2.179986	-0.670138	-1.885093
1	-1.292653	-1.967529	0.732922
1	-4.420579	-0.408606	1.422146
1	-5.062398	-2.198428	-0.306395
1	-1.269494	-2.190373	-1.727429
1	0.245317	-0.036276	-1.608192
6	0.320378	0.157719	1.963431
8	0.273354	0.174880	3.117203

Structure 6 - DIO

B3LYP/GBS(1) = -1464.341427 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.659967 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.439454 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.748178 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.792404 a.u.
Enthalpy Correction = 0.367247

Gibbs Free Energy Correction = 0.29262

Atomic No	x-coord	y-coord	z-coord
7	2.322160	0.787678	-0.043961
6	3.342406	-0.105801	-0.070650
6	3.135086	-1.452699	-0.057272
1	4.357784	0.300191	-0.104086
1	3.964789	-2.152840	-0.077808
6	2.548319	2.126998	-0.059169
6	1.540334	3.044807	-0.040281
1	3.593171	2.450219	-0.087936
1	1.749990	4.110007	-0.052831
15	1.429089	-1.994254	0.005910
15	-0.123732	2.381769	0.002465
6	1.316745	-3.127840	1.469452
1	0.332185	-3.605362	1.528996
1	2.078526	-3.914145	1.411579
1	1.474269	-2.537462	2.375305
6	1.221188	-3.193390	-1.393084
1	1.990960	-3.973143	-1.356341
1	0.237594	-3.674237	-1.353258
1	1.307242	-2.645737	-2.334939
6	-0.984657	3.136541	1.452895
1	-0.996900	4.230606	1.385369
1	-2.013264	2.765573	1.498933
1	-0.460845	2.832970	2.362449
6	-1.049431	3.117674	-1.417886
1	-2.077954	2.743154	-1.414953
1	-1.063378	4.212425	-1.362516
1	-0.564389	2.805464	-2.345833
77	0.283887	0.079532	0.007728
6	-3.951378	0.074796	0.157622
6	-4.210068	-1.298321	-0.417540
6	-2.008043	-1.937282	-0.008243
6	-1.554772	-0.480496	0.050909
1	-4.237268	0.104818	1.214529
1	-4.016183	-1.312965	-1.503259
1	0.387219	0.117576	-1.672711
8	-2.545008	0.425122	0.077832
8	-3.375354	-2.215739	0.260979
1	-1.740098	-2.302744	-1.013748
1	-4.477513	0.867231	-0.382084
1	-5.247022	-1.602151	-0.244447
1	-1.434875	-2.508115	0.722490
1	0.449708	0.133235	1.683106

Structure 7 - DIO

B3LYP/GBS(1) = -1464.331670 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.650362 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.428664 a.u.

TPSS/GBS(2)//B3LYP/GBS(1) = -1464.739297 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.782922 a.u.
Enthalpy Correction = 0.368193
Gibbs Free Energy Correction = 0.293646

Atomic No	x-coord	y-coord	z-coord
7	0.534958	-0.869671	1.646381
6	-0.430516	-1.568800	2.295309
6	-1.566880	-2.008908	1.676180
1	-0.261306	-1.783808	3.355494
1	-2.319795	-2.567038	2.225337
6	1.735784	-0.585827	2.212353
6	2.763537	-0.025006	1.509748
1	1.859367	-0.836292	3.270966
1	3.709024	0.208193	1.991111
15	-1.691285	-1.696668	-0.088165
15	2.465950	0.272010	-0.235998
6	-3.382757	-1.002898	-0.394007
1	-3.577772	-0.957547	-1.471260
1	-4.146766	-1.637181	0.070188
1	-3.459190	0.007853	0.015598
6	-1.829165	-3.331929	-0.938096
1	-2.691444	-3.899114	-0.568404
1	-1.933180	-3.178405	-2.017298
1	-0.911775	-3.895383	-0.754967
6	2.955714	2.028278	-0.569635
1	3.984700	2.215460	-0.241094
1	2.884457	2.238647	-1.642231
1	2.283833	2.698171	-0.027371
6	3.755759	-0.636843	-1.196554
1	3.623029	-0.440749	-2.265727
1	4.764601	-0.331000	-0.895345
1	3.627455	-1.707087	-1.021488
77	0.249240	-0.419113	-0.450251
6	-2.398689	3.345632	0.667523
6	-0.898388	3.500320	0.821232
6	-0.599281	1.356206	-0.210418
6	-1.625249	1.962589	-1.150156
1	-2.878590	4.332142	0.617881
1	-0.627237	3.929580	1.787480
1	-2.051538	1.188841	-1.784668
8	-2.724290	2.621697	-0.512155
8	-0.274365	2.192832	0.780964
1	-1.079598	2.662343	-1.811823
1	-2.797711	2.813929	1.542964
1	-0.472472	4.120724	0.023735
1	0.081358	-0.267477	-2.059213
1	0.944416	-1.898617	-0.824145

Structure 7-8TS - DIO
B3LYP/GBS(1) = -1464.292514a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.614230 a.u.

BMK/GBS(2)//B3LYP/GBS(1) = -1463.385632 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.702966 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.751121 a.u.
Enthalpy Correction = 0.364208
Gibbs Free Energy Correction = 0.289944
Imaginary Freq = -873.7 i

Atomic No	x-coord	y-coord	z-coord
7	-1.696407	1.385031	-0.842945
6	-2.918244	0.870401	-1.129265
6	-3.285579	-0.390501	-0.767097
1	-3.616060	1.518725	-1.668180
1	-4.265254	-0.785353	-1.020348
6	-1.387820	2.676365	-1.129262
6	-0.203598	3.243400	-0.766895
1	-2.142091	3.258225	-1.668048
1	0.029533	4.272234	-1.025323
15	-2.067488	-1.370498	0.111402
15	0.956884	2.185503	0.099624
6	-2.102723	-3.004456	-0.777263
1	-1.545336	-3.774040	-0.234192
1	-3.143727	-3.333996	-0.874524
1	-1.681555	-2.893777	-1.780573
6	-2.837343	-1.883223	1.719908
1	-3.798082	-2.384575	1.554869
1	-2.168963	-2.565281	2.257063
1	-2.998655	-0.994488	2.334825
6	2.537887	2.336846	-0.851042
1	2.732862	3.393663	-1.067079
1	3.373786	1.922417	-0.283568
1	2.442239	1.791181	-1.793024
6	1.409762	3.039749	1.678395
1	2.173461	2.459044	2.206524
1	1.795291	4.047891	1.486966
1	0.520916	3.110099	2.310649
77	-0.255947	0.176285	0.283601
6	3.525403	-2.708004	-0.119560
6	3.692838	-1.226082	-0.364642
6	1.262166	-0.969539	-0.052967
6	1.204263	-2.488845	-0.237869
1	3.462519	-2.920308	0.961644
1	3.839610	-1.041972	-1.436761
1	-1.166907	0.856476	1.688043
1	0.389355	-2.741808	-0.909254
8	2.352632	-3.127473	-0.786663
8	2.534806	-0.486950	0.071699
1	-0.355499	0.250169	1.958594
1	0.981706	-2.924403	0.754957
1	4.364360	-3.273104	-0.538938
1	4.536762	-0.802538	0.188667

Structure 8 - DIO

B3LYP/GBS(1) = -1463.148339 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1463.456052 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1462.231991 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1463.539829 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1463.586697 a.u.
Enthalpy Correction = 0.350982
Gibbs Free Energy Correction = 0.276108

Atomic No	x-coord	y-coord	z-coord
7	2.275310	0.838121	0.000895
6	3.337118	-0.024483	0.015487
6	3.176334	-1.374673	0.028961
1	4.337340	0.418949	0.016552
1	4.028890	-2.047097	0.038691
6	2.479784	2.193489	-0.008464
6	1.455755	3.089253	-0.015969
1	3.519406	2.534670	-0.010575
1	1.643166	4.158698	-0.023707
15	1.473168	-1.952185	0.015312
15	-0.190806	2.364314	-0.004627
6	1.341273	-3.127199	1.446019
1	0.365149	-3.624292	1.447104
1	2.125446	-3.892042	1.402028
1	1.445325	-2.562037	2.376247
6	1.385755	-3.124267	-1.422583
1	2.190135	-3.867013	-1.367861
1	0.426194	-3.652214	-1.443176
1	1.490187	-2.553304	-2.349219
6	-1.086126	3.103633	1.436639
1	-1.115222	4.197468	1.370646
1	-2.108036	2.713337	1.463168
1	-0.575479	2.812522	2.358456
6	-1.104878	3.098287	-1.436224
1	-2.128483	2.711768	-1.445218
1	-1.129591	4.192535	-1.376025
1	-0.609117	2.800278	-2.363942
77	0.289008	0.089151	0.003330
6	-4.162784	-1.426195	0.385293
6	-3.938384	-0.013933	-0.104156
6	-1.518785	-0.515397	-0.041429
6	-1.947816	-1.981742	-0.083940
1	-5.193968	-1.743820	0.200568
1	-4.499822	0.725705	0.475192
1	-1.658592	-2.423394	0.887038
8	-3.313509	-2.281124	-0.352600
8	-2.550315	0.372377	0.012506
1	-1.375511	-2.486686	-0.863898
1	-3.960686	-1.502545	1.467453
1	-4.225808	0.064480	-1.159513

Structure 10 - DIO

B3LYP/GBS(1) = -1464.334385 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.654657 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.441361 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.745588 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.787671 a.u.
Enthalpy Correction = 0.368593
Gibbs Free Energy Correction = 0.295824

Atomic No	x-coord	y-coord	z-coord
7	-0.363174	-2.215170	-0.383337
6	-1.628413	-2.690743	-0.542942
6	-2.734479	-1.914947	-0.392851
1	-1.715521	-3.747607	-0.804683
1	-3.733885	-2.313736	-0.532693
6	0.700416	-3.051149	-0.539844
6	1.988454	-2.644086	-0.393287
1	0.464167	-4.086128	-0.796895
1	2.820642	-3.326294	-0.533476
15	-2.402019	-0.211781	0.022596
15	2.188122	-0.912611	-0.005190
6	-3.402580	0.182456	1.529562
1	-3.328170	1.247126	1.777515
1	-4.458995	-0.059029	1.365419
1	-3.020729	-0.406189	2.367159
6	-3.220194	0.842087	-1.254989
1	-4.298240	0.647363	-1.293656
1	-3.044588	1.896711	-1.026313
1	-2.772568	0.612811	-2.225054
6	3.284004	-0.802995	1.481055
1	4.217299	-1.353379	1.316211
1	3.531050	0.242534	1.694622
1	2.758032	-1.229979	2.338580
6	3.260580	-0.180620	-1.318601
1	3.407977	0.882511	-1.113302
1	4.231612	-0.687791	-1.358893
1	2.749769	-0.290875	-2.278031
77	-0.051688	-0.199997	0.159076
6	1.378477	3.487492	-0.549533
6	0.009956	3.202748	-1.148300
6	-0.426402	1.965456	0.805834
6	0.941406	1.701770	0.938752
1	1.315135	4.341748	0.139793
1	0.065678	2.365911	-1.852768
1	-1.072245	1.888033	1.669960
8	1.882468	2.346852	0.153841
8	-0.913090	2.876085	-0.104881
1	1.339335	1.389890	1.895305
1	2.110611	3.714844	-1.329050
1	-0.394730	4.089744	-1.643359
1	-0.135244	-0.663537	1.781367
1	0.031907	0.248840	-1.465130

Structure 11 - DIO

B3LYP/GBS(1) = -1464.347029 a.u.

B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.665343 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.448877 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1464.753457 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.796675 a.u.
Enthalpy Correction = 0.369229
Gibbs Free Energy Correction = 0.295308

Atomic No	x-coord	y-coord	z-coord
7	0.055146	-1.418801	1.417814
6	-1.125692	-1.875890	1.914265
6	-2.318934	-1.651756	1.285471
1	-1.090242	-2.442310	2.850864
1	-3.247060	-2.022007	1.712169
6	1.260894	-1.766540	1.940940
6	2.442741	-1.435572	1.337391
1	1.256775	-2.334389	2.877380
1	3.391388	-1.721589	1.783245
15	-2.248804	-0.815684	-0.311041
15	2.328759	-0.616313	-0.264325
6	-3.673843	0.364433	-0.359793
1	-3.756300	0.785065	-1.367430
1	-4.606296	-0.158691	-0.117421
1	-3.521479	1.187606	0.339447
6	-2.797834	-2.042177	-1.584466
1	-3.805711	-2.413534	-1.366275
1	-2.793346	-1.571835	-2.573462
1	-2.096066	-2.879446	-1.593429
6	3.645008	0.685148	-0.298184
1	4.610417	0.254863	-0.007375
1	3.729187	1.083990	-1.314622
1	3.393995	1.510570	0.369525
6	3.003645	-1.795617	-1.522198
1	2.966766	-1.335035	-2.515118
1	4.038848	-2.071376	-1.290479
1	2.381786	-2.693871	-1.531578
77	0.020759	-0.232242	-0.395004
6	0.461305	3.455592	-0.504502
6	-0.884657	3.777275	0.130954
6	-0.757932	1.620243	1.067191
6	0.615951	1.705964	1.037743
1	1.007276	4.368928	-0.755345
1	-1.539946	4.300008	-0.570958
8	1.275761	2.743310	0.429636
8	-1.570756	2.580416	0.509579
1	1.230221	1.182166	1.758092
1	0.323796	2.838485	-1.399607
1	-0.736566	4.407214	1.019484
1	-1.264728	0.992968	1.788826
1	0.085989	-1.462636	-1.407070
1	-0.006445	0.652608	-1.750301

Structure 11-13TS - DIO
B3LYP/GBS(1) = -1464.305428 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.624466 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1463.405377 a.u.

TPSS/GBS(2)//B3LYP/GBS(1) = -1464.714610 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1464.756993 a.u.
Enthalpy Correction = 0.36481
Gibbs Free Energy Correction = 0.291126
Imaginary Freq = -139.9 i

Atomic No	x-coord	y-coord	z-coord
7	-1.171165	1.812721	-0.648983
6	-0.414025	2.924149	-0.869189
6	0.909731	2.983915	-0.552295
1	-0.918933	3.786683	-1.314922
1	1.489126	3.881573	-0.748346
6	-2.493591	1.779903	-0.951363
6	-3.277742	0.687881	-0.706443
1	-2.923886	2.678309	-1.404796
1	-4.333184	0.685605	-0.961838
15	1.639817	1.495511	0.147006
15	-2.459541	-0.716926	0.046393
6	2.394530	1.957666	1.774386
1	2.864416	1.069655	2.209169
1	3.147365	2.745073	1.654329
1	1.615052	2.313374	2.453373
6	3.154295	1.160391	-0.851098
1	3.765331	2.068566	-0.910797
1	3.735067	0.364722	-0.377626
1	2.863263	0.837676	-1.851357
6	-3.386291	-1.126017	1.599320
1	-4.451372	-1.283217	1.393799
1	-2.974857	-2.033076	2.055745
1	-3.280901	-0.300017	2.307932
6	-2.867648	-2.193970	-0.995482
1	-2.449755	-3.106433	-0.556123
1	-3.953979	-2.311020	-1.079523
1	-2.450334	-2.059996	-1.997178
77	-0.244232	0.070105	0.249833
6	2.725349	-2.365456	-1.245677
6	2.858669	-2.616120	0.284595
6	0.758740	-1.716528	0.643949
6	0.556833	-1.554566	-0.788721
1	2.505985	-3.310430	-1.767372
1	3.902396	-2.538871	0.605697
8	1.723502	-1.391414	-1.549870
8	2.128529	-1.643817	1.023914
1	-0.191768	-2.146549	-1.319402
1	3.652330	-1.961152	-1.663537
1	2.500211	-3.625894	0.541001
1	0.233688	-2.508617	1.188829
1	-0.867988	1.212024	1.971397
1	-0.506724	0.530523	2.132031

Structure 12 - DIO

B3LYP/GBS(1) = -306.427911 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -306.533672 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -306.350457 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -306.578399 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -306.532396 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -306.3352172 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -305.7470619 a.u.
Enthalpy Correction = 0.105121
Gibbs Free Energy Correction = 0.071021

Atomic No	x-coord	y-coord	z-coord
6	0.665283	1.192546	-0.079283
6	-0.664150	1.193164	0.079298
8	-1.427790	0.050763	0.138928
6	-0.704010	-1.097820	-0.297638
6	0.702979	-1.098448	0.297683
8	1.427825	0.049403	-0.139010
1	-1.274613	-1.972632	0.026521
1	0.637581	-1.095894	1.394706
1	1.272750	-1.973833	-0.026388
1	-0.638612	-1.095442	-1.394660
1	1.250436	2.099329	-0.167269
1	-1.248438	2.100496	0.167390

Structure 13 - DIO

B3LYP/GBS(1) = -1463.146454 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1463.457448 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1462.239989 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1463.543272 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1463.589056 a.u.
Enthalpy Correction = 0.350773
Gibbs Free Energy Correction = 0.277723

Atomic No	x-coord	y-coord	z-coord
7	1.281112	1.876417	-0.057398
6	0.593440	3.064688	-0.119582
6	-0.761528	3.121440	-0.119562
1	1.196536	3.975222	-0.168692
1	-1.288608	4.069664	-0.161053
6	2.650512	1.877233	-0.056871
6	3.391094	0.736574	-0.014214
1	3.137390	2.855577	-0.094125
1	4.476080	0.764723	-0.014884
15	-1.589265	1.526051	0.001449
15	2.430154	-0.775841	0.031383
6	-2.850468	1.516316	-1.350969
1	-3.418698	0.583225	-1.330231

1	-3.533826	2.368272	-1.259064
1	-2.329195	1.571831	-2.310261
6	-2.616000	1.651662	1.539421
1	-3.356291	2.455746	1.455995
1	-3.121711	0.706739	1.750021
1	-1.945039	1.868277	2.375066
6	3.053061	-1.844307	-1.349117
1	4.134036	-2.005612	-1.268455
1	2.550926	-2.818286	-1.332365
1	2.833650	-1.355580	-2.302297
6	2.991425	-1.728153	1.519109
1	2.484936	-2.699183	1.562520
1	4.073797	-1.898342	1.497281
1	2.735228	-1.161382	2.418276
77	0.239622	0.063193	-0.013603
6	-3.106387	-1.923195	0.654074
6	-2.827626	-2.508737	-0.720624
6	-0.646476	-1.735714	-0.695056
6	-0.698098	-1.732474	0.727753
1	-3.744825	-2.591849	1.245235
1	-3.739044	-2.505973	-1.326561
8	-1.912988	-1.708369	1.414509
8	-1.867247	-1.700874	-1.396649
1	0.032768	-2.281192	1.317961
1	-3.636373	-0.969238	0.535718
1	-2.464049	-3.544820	-0.639968
1	0.094508	-2.339790	-1.222427

4.3. Coordinates of DIO structures at the Full-opt level of theory

Full Structure 5 - DIO
B3LYP/GBS(1) = -2164.750240 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2165.259150 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2164.099709 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -2160.065849 a.u.
Enthalpy Correction = 0.771459
Gibbs Free Energy Correction = 0.654029

Atomic No	x-coord	y-coord	z-coord
77	-0.068184	-0.553095	0.132111
6	-2.205729	-4.286272	0.386060
6	-2.403119	-4.609576	-1.091833
6	-0.908156	-2.882319	-1.640082
6	-0.657536	-2.565896	-0.166205
1	-1.404937	-4.925077	0.795334
1	-3.282362	-4.059685	-1.472676
1	-0.015502	-2.713525	-2.246275
8	-1.871480	-2.914294	0.560480
8	-1.248449	-4.264888	-1.838571
1	0.116459	-3.268485	0.184962
1	-3.124928	-4.469443	0.955720
1	-2.573108	-5.681815	-1.243940
1	-0.137552	-1.269133	1.519473
1	-1.719642	-2.253559	-2.036180
15	-2.171572	0.380318	0.529595
6	-1.889469	2.097922	-0.043567
6	-3.634046	-0.280591	-0.457839
6	-2.739603	0.507476	2.312381
6	-2.908040	3.051208	-0.174804
6	-0.573566	2.384014	-0.499590
6	-3.447674	0.031486	-1.953071
6	-5.040181	0.127804	0.009198
1	-3.515735	-1.359983	-0.309657
1	-3.656746	1.112532	2.294349
6	-1.689792	1.252658	3.151489
6	-3.060890	-0.870002	2.914225
6	-2.713297	4.274026	-0.822255
1	-3.893824	2.830484	0.226885
6	-0.411191	3.578056	-1.240997
7	0.454010	1.452030	-0.265658
1	-3.623901	1.091445	-2.162155
1	-4.159508	-0.554544	-2.547624
1	-2.438547	-0.212122	-2.301223
1	-5.227637	1.196824	-0.136155
1	-5.787697	-0.412824	-0.585762
1	-5.225425	-0.112908	1.060057
1	-1.499150	2.258044	2.763802
1	-2.040495	1.346570	4.186897
1	-0.739078	0.709656	3.159792
1	-3.857911	-1.388061	2.372257
1	-3.384926	-0.749070	3.955774
1	-2.183899	-1.522927	2.894438
6	-3.813467	5.303833	-0.926050
6	-1.449407	4.490151	-1.389799

1	0.538220	3.782444	-1.721477
6	1.794470	1.848777	-0.150013
1	-3.867103	5.737689	-1.931940
1	-4.792440	4.868106	-0.698499
1	-3.657258	6.136497	-0.226395
1	-1.271175	5.394982	-1.968253
6	2.228698	3.183143	0.047895
6	2.815816	0.855971	-0.144622
1	1.498559	3.971300	0.179015
6	3.576979	3.513470	0.104242
6	4.168922	1.222030	-0.130046
15	2.247009	-0.878772	-0.029165
1	3.850226	4.556146	0.257813
6	4.587162	2.550482	-0.029234
1	4.926502	0.444525	-0.186877
6	3.110136	-1.759575	-1.451069
6	3.011235	-1.613240	1.535007
6	6.048605	2.931616	-0.040024
6	2.664709	-1.169174	-2.798805
1	4.178792	-1.537549	-1.327317
6	2.925744	-3.285614	-1.407745
6	4.527417	-1.868670	1.509554
1	2.497597	-2.581109	1.617894
6	2.638723	-0.768546	2.765132
1	6.338477	3.407789	-0.986744
1	6.286701	3.642927	0.760579
1	6.691581	2.054649	0.092770
1	3.223417	-1.642412	-3.615834
1	2.845279	-0.090708	-2.844981
1	1.598422	-1.340599	-2.980859
1	3.471750	-3.746764	-2.240204
1	1.875021	-3.573808	-1.503600
1	3.307503	-3.726310	-0.480971
1	4.852046	-2.468169	0.653916
1	5.088958	-0.929211	1.504191
1	4.816309	-2.412459	2.417870
1	3.123196	0.213281	2.727473
1	1.559447	-0.611206	2.836622
1	2.975247	-1.275951	3.677855

Full Structure 6 - DIO

B3LYP/GBS(1) = -2164.733092 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2165.245729 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2164.079674 a.u.
MP2/GBS(2)//B3LYP/GBS(1) = -2160.059068 a.u.
Enthalpy Correction = 0.767549
Gibbs Free Energy Correction = 0.649432

Atomic No	x-coord	y-coord	z-coord
1	0.045880	-0.613994	0.006194
2	1.858578	-4.457015	0.030208
3	0.634423	-5.315500	0.241332
4	-0.766027	-3.550324	-0.343109
5	0.325038	-2.521380	-0.056971
6	2.267185	-4.615941	-0.973224

7	0.278821	-5.249542	1.283423
8	0.333902	-0.465431	1.655242
9	1.542913	-3.044417	0.147213
10	-0.356896	-4.872768	-0.663297
11	-1.423732	-3.570204	0.542039
12	2.640752	-4.639351	0.772645
13	0.850717	-6.363639	0.013032
14	-1.346278	-3.200981	-1.195987
15	-0.283570	-0.543582	-1.642794
16	2.292299	-0.003588	-0.304990
17	2.226158	1.784764	0.028595
18	3.576125	-0.745711	0.876249
19	3.043235	-0.172103	-2.024418
20	3.372708	2.582201	0.170760
21	0.929319	2.341801	0.200118
22	3.370277	-0.233426	2.310784
23	5.052510	-0.625598	0.458499
24	3.310285	-1.806207	0.863133
25	4.066589	0.218544	-1.944566
26	2.283705	0.686232	-3.046641
27	3.101902	-1.638658	-2.477554
28	3.312082	3.920808	0.554562
29	4.349036	2.142809	-0.015478
30	0.883977	3.684030	0.668178
31	-0.185562	1.554430	-0.021324
32	3.646287	0.822109	2.403491
33	4.001775	-0.810311	2.998887
34	2.329083	-0.341120	2.626151
35	5.404269	0.410918	0.460480
36	5.672343	-1.173471	1.180163
37	5.252294	-1.050676	-0.529631
38	2.296478	1.745279	-2.772548
39	2.752422	0.583378	-4.033815
40	1.239315	0.368135	-3.125104
41	3.666933	-2.271983	-1.784706
42	3.582432	-1.708308	-3.461493
43	2.090220	-2.048606	-2.566791
44	4.553217	4.771150	0.688886
45	2.034722	4.437509	0.834137
46	-0.072574	4.123777	0.924224
47	-1.425857	2.092031	-0.302315
48	4.597327	5.274441	1.663445
49	5.462424	4.168390	0.587124
50	4.595146	5.557584	-0.077239
51	1.941991	5.458480	1.201442
52	-1.635890	3.379138	-0.868619
53	-2.590524	1.306583	-0.080836
54	-0.779442	3.971439	-1.167839
55	-2.908743	3.886437	-1.072509
56	-3.867192	1.863604	-0.256007
57	-2.298095	-0.429557	0.399614
58	-3.012629	4.876384	-1.514206
59	-4.062588	3.159036	-0.733912
60	-4.743340	1.269653	-0.015702
61	-2.914248	-0.562208	2.174596
62	-3.519951	-1.493546	-0.593089
63	-5.443203	3.748497	-0.901543
64	-2.253014	0.488915	3.077064
65	-3.989422	-0.344474	2.131798
66	-2.708789	-1.977594	2.734690
67	-4.998495	-1.484285	-0.161585

68	-3.160275	-2.511268	-0.412088
69	-3.387035	-1.207616	-2.097987
70	-5.628940	4.563957	-0.188940
71	-5.587396	4.166117	-1.906436
72	-6.221332	2.993770	-0.742637
73	-2.661945	0.411095	4.092697
74	-2.437407	1.503856	2.712826
75	-1.170529	0.337144	3.126351
76	-3.089003	-2.037459	3.762193
77	-1.641147	-2.224877	2.758500
78	-3.230051	-2.744241	2.148722
79	-5.134484	-1.706961	0.900852
80	-5.491813	-0.533031	-0.378425
81	-5.534775	-2.257342	-0.726887
82	-3.773404	-0.212691	-2.342281
83	-2.344327	-1.245291	-2.428040
84	-3.963727	-1.945692	-2.669749

Full Structure 7 - DIO

B3LYP/GBS(1) = -2164.727650 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2165.239869 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2164.076044 a.u.
Enthalpy Correction = 0.768099
Gibbs Free Energy Correction = 0.651626

Atomic No	x-coord	y-coord	z-coord
77	0.049192	-0.784860	0.606988
6	-1.031542	-3.216687	-3.405495
6	-1.208961	-1.714202	-3.419547
6	-0.518802	-1.736727	-1.059015
6	-0.812429	-3.230769	-1.089763
1	0.032275	-3.489141	-3.507061
1	-2.268414	-1.445534	-3.468710
1	0.445502	-0.120775	2.075622
1	-1.358330	-3.496966	-0.184408
8	-1.564143	-3.719530	-2.194203
8	-0.681685	-1.097243	-2.208187
1	0.009592	-2.194151	1.405770
1	0.164025	-3.742091	-1.036649
1	-1.585202	-3.677438	-4.229485
1	-0.676381	-1.230028	-4.242084
15	-2.078187	-0.001048	1.189152
6	-2.293614	1.321586	-0.055501
6	-3.566529	-1.179341	1.109355
6	-2.247732	0.824813	2.871231
6	-3.532653	1.903784	-0.360351
6	-1.109687	1.726173	-0.748111
6	-3.961568	-1.532497	-0.334355
6	-4.818272	-0.766081	1.906211
1	-3.161289	-2.086901	1.577608
1	-3.296040	1.144671	2.934021
6	-1.369263	2.078855	2.979652
6	-1.951022	-0.164801	4.008889
6	-3.693934	2.839817	-1.382889
1	-4.409098	1.610622	0.212289

6	-1.302721	2.623900	-1.833068
7	0.106341	1.178021	-0.385121
1	-4.373151	-0.665022	-0.859139
1	-4.730254	-2.315259	-0.320131
1	-3.126110	-1.914414	-0.924216
1	-5.276354	0.148049	1.513585
1	-5.570124	-1.561890	1.830316
1	-4.614483	-0.612058	2.968929
1	-1.629530	2.821054	2.219293
1	-1.509028	2.538062	3.966666
1	-0.310791	1.829139	2.863655
1	-2.599880	-1.047581	3.982509
1	-2.097183	0.326289	4.979216
1	-0.914723	-0.511584	3.949102
6	-5.033446	3.469531	-1.684697
6	-2.548078	3.156588	-2.131368
1	-0.460557	2.872616	-2.467734
6	1.326088	1.786291	-0.569505
1	-5.279166	3.411625	-2.752946
1	-5.840202	2.974849	-1.132571
1	-5.055819	4.533402	-1.410903
1	-2.636913	3.833642	-2.979864
6	1.510500	3.161618	-0.901161
6	2.530451	1.045348	-0.340681
1	0.648127	3.813559	-0.960319
6	2.765799	3.705818	-1.112814
6	3.786743	1.621619	-0.594732
15	2.366560	-0.618610	0.385952
1	2.838150	4.763729	-1.361746
6	3.943059	2.943463	-1.005573
1	4.680366	1.017162	-0.452264
6	3.346744	-1.776264	-0.731995
6	3.344464	-0.641485	2.016648
6	5.300177	3.538790	-1.296230
6	2.918498	-1.646996	-2.199538
1	4.393539	-1.454127	-0.663300
6	3.248036	-3.229743	-0.240755
6	4.860783	-0.878595	1.899931
1	2.897373	-1.490861	2.549073
6	3.088264	0.628437	2.843731
1	5.444011	3.730201	-2.368920
1	5.442142	4.497858	-0.781427
1	6.105912	2.869271	-0.974950
1	3.522143	-2.317864	-2.824487
1	3.047986	-0.625292	-2.567670
1	1.866735	-1.915549	-2.332811
1	3.846437	-3.888886	-0.882521
1	2.211295	-3.580253	-0.264057
1	3.606418	-3.351141	0.786616
1	5.118382	-1.818003	1.403305
1	5.359075	-0.060946	1.367853
1	5.294905	-0.915889	2.907050
1	3.525550	1.508424	2.360369
1	2.020993	0.810494	2.984014
1	3.550820	0.518630	3.832847

Full Structure 7-8TS - DIO

B3LYP/GBS(1) = -2164.679140 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2165.194550 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2164.033977 a.u.
Enthalpy Correction = 0.764198
Gibbs Free Energy Correction = 0.648084
Imaginary Freq = -966.2 i

Atomic No	x-coord	y-coord	z-coord
77	-0.443290	3.133349	2.483888
6	3.045842	0.064285	3.233937
6	3.444350	1.440336	2.757755
6	1.027002	1.857565	2.382879
6	0.905957	0.332450	2.324727
1	2.627795	0.104949	4.254232
1	3.924382	1.367585	1.774133
1	-1.271451	3.898518	3.850163
1	0.393423	0.057644	1.405074
8	2.102208	-0.440011	2.312535
8	2.294430	2.302597	2.642539
1	-0.479383	3.171140	4.132343
1	0.274303	0.021673	3.174396
1	3.903616	-0.615953	3.235234
1	4.123788	1.948994	3.449471
15	-2.353308	1.727972	2.207507
6	-3.482546	2.827089	1.283948
6	-2.239558	0.153496	1.146179
6	-3.334926	1.159708	3.713875
6	-4.760855	2.415890	0.865265
6	-2.999113	4.117576	0.935930
6	-1.665658	0.506833	-0.236500
6	-3.502303	-0.712133	0.990174
1	-1.509089	-0.461267	1.681737
1	-4.227930	0.662971	3.312884
6	-3.809326	2.338890	4.574909
6	-2.545419	0.141164	4.551910
6	-5.561308	3.183329	0.021765
1	-5.148366	1.463032	1.212765
6	-3.779482	4.848062	-0.003773
7	-1.806748	4.573807	1.458990
1	-2.390516	1.089263	-0.815310
1	-1.442142	-0.408965	-0.798219
1	-0.750924	1.103950	-0.162232
1	-4.255565	-0.224919	0.365603
1	-3.227630	-1.650783	0.491709
1	-3.963218	-0.978457	1.946867
1	-4.375925	3.066710	3.986379
1	-4.458714	1.968911	5.378479
1	-2.966306	2.862731	5.035991
1	-2.267531	-0.750407	3.978365
1	-3.148002	-0.193010	5.405820
1	-1.627594	0.590582	4.948864
6	-6.939994	2.732235	-0.399564
6	-5.012579	4.393686	-0.439403
1	-3.390395	5.780492	-0.396599
6	-1.573568	5.917460	1.701975
1	-7.055519	2.743938	-1.491230
1	-7.148091	1.712977	-0.056121
1	-7.725213	3.382235	0.010118

1	-5.568609	4.993081	-1.158640
6	-2.570933	6.929167	1.735851
6	-0.251346	6.335371	2.028432
1	-3.610947	6.659315	1.601849
6	-2.253780	8.258192	1.974537
6	0.044135	7.690690	2.230181
15	0.972469	4.989925	2.164296
1	-3.061030	8.988858	1.998693
6	-0.934503	8.684626	2.195906
1	1.069067	7.985493	2.434901
6	1.922917	5.141827	0.538381
6	2.215526	5.407726	3.523342
6	-0.600329	10.142638	2.406124
6	0.962665	5.021386	-0.656013
1	2.312843	6.169310	0.559006
6	3.099695	4.170843	0.371976
6	3.302066	6.448996	3.197786
1	2.711993	4.440815	3.658809
6	1.500801	5.756917	4.839268
1	-0.740284	10.731170	1.488884
1	-1.236149	10.598611	3.176057
1	0.441566	10.271709	2.719547
1	1.523784	5.146163	-1.590963
1	0.178293	5.781890	-0.626191
1	0.480955	4.038512	-0.670436
1	3.649147	4.419246	-0.545186
1	2.739220	3.142635	0.280230
1	3.807197	4.206791	1.206116
1	3.845432	6.226239	2.275250
1	2.897990	7.462608	3.115433
1	4.036047	6.464113	4.013901
1	0.957360	6.704227	4.762290
1	0.785018	4.982604	5.128681
1	2.239243	5.854481	5.645154

Full Structure 8 - DIO

B3LYP/GBS(1) = -2163.548737 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2164.050290 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2162.897189 a.u.
Enthalpy Correction = 0.750776
Gibbs Free Energy Correction = 0.632671

Atomic No	x-coord	y-coord	z-coord
77	0.051034	-0.588748	0.006360
6	0.911890	-5.235025	-0.482269
6	1.987071	-4.351547	0.105813
6	0.369885	-2.473577	-0.001899
6	-0.685840	-3.571988	-0.133472
1	1.120591	-6.291678	-0.286167
1	2.952064	-4.470932	-0.396722
1	-1.065372	-3.517558	-1.171182
8	-0.306020	-4.913280	0.156921
8	1.652737	-2.953456	-0.026723
1	-1.515680	-3.360262	0.536585
1	0.836408	-5.087780	-1.573472

1	2.108578	-4.575130	1.172823
15	2.288187	0.024248	-0.259760
6	2.194761	1.833116	-0.017910
6	3.470183	-0.631467	1.056791
6	3.180098	-0.172261	-1.904532
6	3.315097	2.671751	0.068880
6	0.886793	2.354007	0.172408
6	2.915487	-0.306670	2.454005
6	4.950470	-0.235080	0.944019
1	3.390014	-1.712876	0.908832
1	4.104680	0.414257	-1.813818
6	2.330617	0.438463	-3.030655
6	3.551018	-1.627083	-2.224253
6	3.219534	4.015934	0.434021
1	4.299031	2.265743	-0.149461
6	0.807835	3.692088	0.635093
7	-0.217029	1.518782	-0.032872
1	2.936519	0.771692	2.647858
1	3.524878	-0.798935	3.223086
1	1.880651	-0.649374	2.556564
1	5.106953	0.818873	1.192132
1	5.538175	-0.825099	1.659486
1	5.367636	-0.420105	-0.051640
1	2.100689	1.491034	-2.839091
1	2.870839	0.375570	-3.984054
1	1.381823	-0.099021	-3.136643
1	4.192774	-2.073962	-1.457323
1	4.091493	-1.669923	-3.178532
1	2.653201	-2.245944	-2.312728
6	4.433705	4.912015	0.503542
6	1.938395	4.488667	0.757438
1	-0.154154	4.105091	0.913343
6	-1.483528	2.054120	-0.277369
1	4.493643	5.440790	1.463457
1	5.359587	4.338896	0.383130
1	4.420127	5.679454	-0.282482
1	1.820888	5.510015	1.116212
6	-1.723882	3.338009	-0.829461
6	-2.628604	1.252020	-0.028560
1	-0.886526	3.942516	-1.156482
6	-3.010443	3.837151	-0.977019
6	-3.915087	1.799836	-0.136235
15	-2.283990	-0.508422	0.333355
1	-3.140062	4.829690	-1.405641
6	-4.140822	3.101395	-0.589042
1	-4.774315	1.195493	0.138160
6	-3.021400	-0.764750	2.048633
6	-3.385149	-1.503476	-0.845782
6	-5.531219	3.684824	-0.680164
6	-2.288309	0.124397	3.065832
1	-4.064211	-0.425161	1.982365
6	-3.007879	-2.232484	2.497131
6	-4.910396	-1.413083	-0.670760
1	-3.102857	-2.540649	-0.634140
6	-2.979266	-1.195885	-2.297202
1	-5.693035	4.472884	0.068124
1	-5.717700	4.136617	-1.662858
1	-6.297305	2.918882	-0.517044
1	-2.744230	0.012147	4.057904
1	-2.336269	1.181442	2.787331
1	-1.231994	-0.156864	3.138515

1	-3.485562	-2.327770	3.480362
1	-1.980100	-2.599894	2.594850
1	-3.546820	-2.892300	1.807639
1	-5.232243	-1.556691	0.366142
1	-5.302696	-0.455815	-1.024096
1	-5.387538	-2.197990	-1.271780
1	-3.232078	-0.163699	-2.563568
1	-1.901967	-1.324662	-2.445997
1	-3.511750	-1.862923	-2.987197

Full Structure 13 - DIO

B3LYP/GBS(1) = -2163.545040 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2164.049350 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2162.904726 a.u.
Enthalpy Correction = 0.750724
Gibbs Free Energy Correction = 0.635652

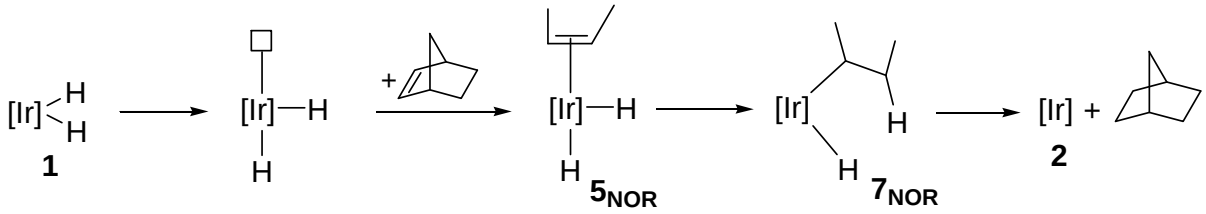
Atomic No	x-coord	y-coord	z-coord
77	-0.047175	-0.667520	-0.065793
6	-2.379770	-3.891359	0.667109
6	-2.141861	-4.119610	-0.817868
6	-0.424426	-2.578898	-0.894321
6	-0.247349	-2.745143	0.510171
1	-2.546229	-4.845014	1.185509
1	-3.076675	-4.402909	-1.311673
8	-1.280747	-3.238308	1.313808
8	-1.692119	-2.907018	-1.420074
1	0.703388	-3.085903	0.911699
1	-3.275816	-3.274650	0.803165
1	-1.403855	-4.919188	-0.984503
1	0.365979	-2.858876	-1.590478
15	-2.220727	0.145361	0.359871
6	-1.986974	1.914692	-0.048958
6	-3.646656	-0.471207	-0.708727
6	-2.857566	0.223460	2.134217
6	-3.027021	2.839420	-0.209415
6	-0.643006	2.301457	-0.274883
6	-3.344632	-0.179640	-2.188388
6	-5.072248	-0.031203	-0.334588
1	-3.575638	-1.555282	-0.577833
1	-3.701389	0.926737	2.099268
6	-1.769941	0.819698	3.043041
6	-3.349546	-1.118821	2.690775
6	-2.810318	4.137777	-0.677082
1	-4.043748	2.540180	0.026556
6	-0.436790	3.589389	-0.825697
7	0.379890	1.379819	-0.013447
1	-3.391442	0.893912	-2.399740
1	-4.084539	-0.683643	-2.822946
1	-2.353301	-0.546728	-2.465816

1	-5.253515	1.019741	-0.577438
1	-5.792640	-0.620794	-0.916493
1	-5.306107	-0.181015	0.723817
1	-1.439601	1.802953	2.694958
1	-2.159915	0.932490	4.062748
1	-0.893878	0.163337	3.080316
1	-4.175626	-1.536682	2.104809
1	-3.715457	-0.978873	3.716110
1	-2.538572	-1.851880	2.712478
6	-3.940767	5.128279	-0.829592
6	-1.491337	4.472521	-1.017320
1	0.560924	3.892511	-1.120131
6	1.687004	1.816116	0.219850
1	-3.922003	5.616188	-1.812259
1	-4.915756	4.640990	-0.720081
1	-3.888202	5.926208	-0.076163
1	-1.281853	5.450651	-1.447233
6	2.021356	3.097384	0.727488
6	2.770982	0.924919	0.005917
1	1.230589	3.779726	1.015492
6	3.341549	3.498168	0.876129
6	4.096508	1.368853	0.122567
15	2.292179	-0.803361	-0.311387
1	3.543342	4.493120	1.269611
6	4.417631	2.661991	0.536715
1	4.906828	0.683001	-0.109488
6	3.155441	-1.236094	-1.930500
6	3.151983	-1.849418	1.006116
6	5.848015	3.137210	0.635831
6	2.520367	-0.439755	-3.081914
1	4.191513	-0.891967	-1.806901
6	3.185036	-2.740807	-2.242924
6	4.687631	-1.912390	0.966710
1	2.772509	-2.862267	0.807565
6	2.665859	-1.422716	2.402637
1	6.092670	3.860861	-0.153864
1	6.044351	3.633604	1.594515
1	6.553156	2.303980	0.543194
1	3.062424	-0.633369	-4.016306
1	2.549842	0.637315	-2.890122
1	1.472683	-0.724741	-3.227582
1	3.769515	-2.915729	-3.154839
1	2.180021	-3.135931	-2.423537
1	3.640028	-3.332505	-1.441997
1	5.083255	-2.187488	-0.016213
1	5.131572	-0.956448	1.259828
1	5.037857	-2.666166	1.683500
1	3.026643	-0.417721	2.647319
1	1.573447	-1.410277	2.463905
1	3.052700	-2.114176	3.161745

5. [Ir]-H_2 + Norbornylene

5.1. Norbornylene (NOR) relative energy diagrams

Scheme S5



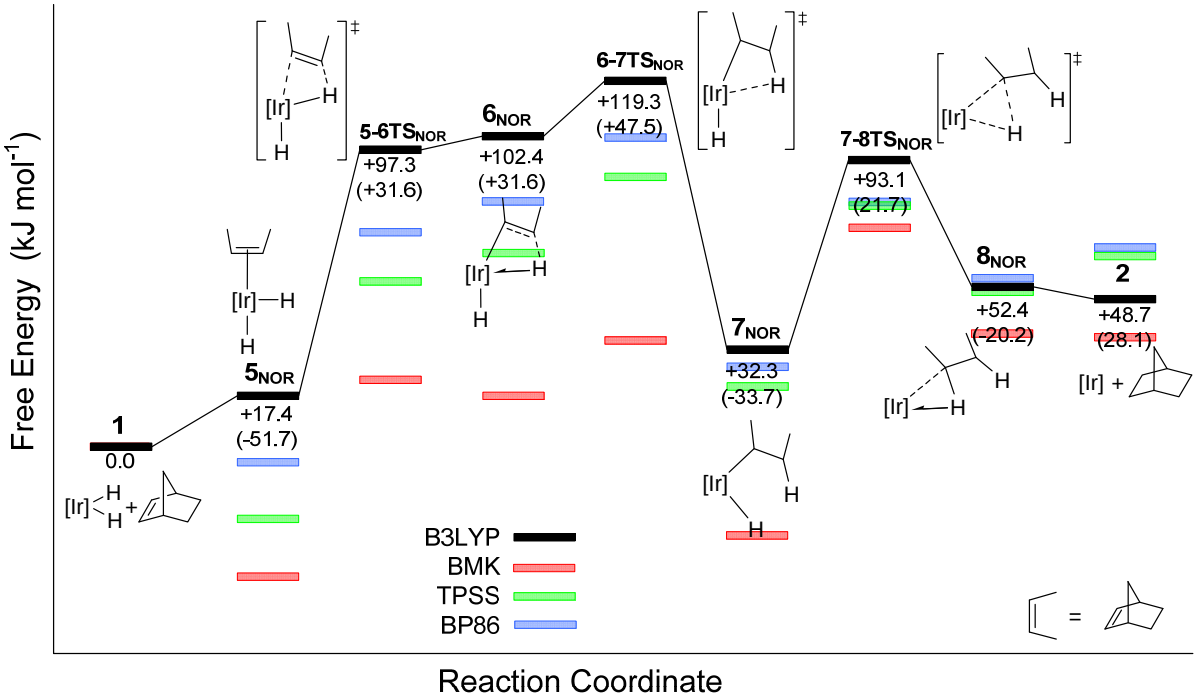


Figure S25. Relative energy surface for the reaction of [Ir]-H_2 + Norbornyle). Values are B3LYP Gibbs corrected Model-opt energies. Drawn to scale with all values in kJ mol^{-1}.

5.2. [Ir]-H2 + Norbornylene structures. Model-opt level of theory.

Structure 3 - NOR

B3LYP/GBS(1) = -1157.855367a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1158.072024 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1157.035198 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1158.105122 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1158.195448 a.u.
Enthalpy Correction = 0.26003
Gibbs Free Energy Correction = 0.198875

Atomic No	x-coord	y-coord	z-coord
7	0.000023	1.576946	-0.000403
6	1.193473	2.244493	0.003920
6	2.399457	1.620661	0.005300
1	1.111990	3.332036	0.006416
1	3.323527	2.189536	0.008901
6	-1.192944	2.244751	-0.003434
6	-2.399276	1.621552	-0.004939
1	-1.111061	3.332275	-0.004732
1	-3.322814	2.191303	-0.007752
15	2.322597	-0.167186	0.000386
15	-2.323279	-0.166128	0.001382
6	3.314272	-0.773266	1.438560
1	3.330268	-1.868842	1.445517
1	4.345949	-0.405421	1.394867
1	2.837567	-0.426777	2.358266
6	3.330555	-0.766954	-1.429522
1	4.363928	-0.405942	-1.368611
1	3.340449	-1.862534	-1.444754
1	2.869519	-0.410486	-2.353461
6	-3.317747	-0.764968	1.440800
1	-4.351376	-0.403042	1.390916
1	-3.328029	-1.860577	1.455200
1	-2.846735	-0.409711	2.360130
6	-3.328156	-0.776183	-1.426222
1	-3.345162	-1.871787	-1.428285
1	-4.359248	-0.407836	-1.373539
1	-2.860842	-0.433642	-2.352171
77	0.000176	-0.432358	-0.003263
1	0.009735	-0.466584	1.689877
1	-0.008963	-0.459843	-1.696013

Structure 4 - NOR

B3LYP/GBS(1) = -1430.630044 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1430.92930 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1429.707180 a.u.

TPSS/GBS(2)//B3LYP/GBS(1) = -1431.027144 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1431.055647 a.u.
Enthalpy Correction = 0.423289
Gibbs Free Energy Correction = 0.349425

Atomic No	x-coord	y-coord	z-coord
7	2.203577	1.069737	-0.000986
6	3.350212	0.340439	-0.001179
6	3.368807	-1.020357	-0.000835
1	4.282757	0.909839	-0.001643
1	4.301497	-1.575028	-0.001030
6	2.257875	2.431432	-0.000626
6	1.145353	3.205415	0.000128
1	3.255897	2.875645	-0.000985
1	1.207465	4.289181	0.000279
15	1.765569	-1.800078	0.000255
15	-0.417385	2.326115	0.000345
6	1.729712	-2.975214	1.431184
1	0.806676	-3.565443	1.425794
1	2.581630	-3.663536	1.389343
1	1.775037	-2.398827	2.358483
6	1.728670	-2.976906	-1.429261
1	2.580914	-3.664817	-1.387462
1	0.805887	-3.567512	-1.422213
1	1.772833	-2.401629	-2.357311
6	-1.335314	3.034920	1.447772
1	-1.374591	4.128027	1.375723
1	-2.356762	2.649108	1.511991
1	-0.797307	2.753341	2.356411
6	-1.335527	3.035658	-1.446644
1	-2.357106	2.650220	-1.510870
1	-1.374447	4.128752	-1.374155
1	-0.797746	2.754301	-2.355490
77	0.335986	0.073106	0.000012
1	0.465287	0.171433	1.669990
1	0.463568	0.170971	-1.670122
6	-1.350011	-1.201859	-0.712079
6	-1.350212	-1.201531	0.712094
6	-2.745522	-0.739324	-1.133076
1	-2.846930	-0.373646	-2.157617
6	-2.745915	-0.738859	1.132407
1	-2.847683	-0.372760	2.156765
6	-3.657691	-1.962394	-0.784167
6	-3.657957	-1.962070	0.783719
6	-3.156697	0.215976	-0.000604
1	-4.231215	0.434831	-0.000848
1	-2.610074	1.150633	-0.000709
1	-4.668078	-1.811213	-1.181714
1	-3.276335	-2.897828	-1.207768
1	-4.668483	-1.810710	1.180843
1	-3.276770	-2.897339	1.207842
1	-0.904407	-1.993160	-1.305128
1	-0.904936	-1.992682	1.305609

Structure 5 - NOR

B3LYP/GBS(1) = -1430.643700 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1430.941441 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1429.717882 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1431.037129 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1431.065870 a.u.
Enthalpy Correction = 0.424545
Gibbs Free Energy Correction = 0.351237

Atomic No	x-coord	y-coord	z-coord
7	1.267755	0.058233	1.601521
6	1.575464	1.263945	2.147107
6	1.389898	2.440213	1.476037
1	1.996148	1.264970	3.158413
1	1.628935	3.391212	1.943764
6	1.683056	-1.114600	2.147872
6	1.604269	-2.303987	1.478443
1	2.103036	-1.076915	3.158770
1	1.929753	-3.228482	1.947065
15	0.820632	2.320140	-0.226557
15	1.025656	-2.237650	-0.223750
6	2.168088	2.981794	-1.309035
1	1.843226	2.959778	-2.354780
1	2.425476	4.010930	-1.033352
1	3.049987	2.345661	-1.204699
6	-0.443725	3.656095	-0.441993
1	-0.006742	4.630398	-0.193801
1	-0.790047	3.679221	-1.480318
1	-1.299943	3.477732	0.211108
6	2.427188	-2.766588	-1.310794
1	2.776419	-3.771626	-1.047678
1	2.101897	-2.760459	-2.356627
1	3.248225	-2.054869	-1.198080
6	-0.113092	-3.681091	-0.442549
1	-0.472577	-3.719613	-1.475816
1	0.415167	-4.614885	-0.217288
1	-0.971489	-3.591698	0.225972
77	0.407864	0.015437	-0.402026
1	1.832199	0.078468	-1.141610
1	-0.156259	-0.018235	-1.909349
6	-1.634598	0.627915	0.613515
1	-1.314718	1.233433	1.456593
6	-1.574411	-0.766980	0.620644
1	-1.203032	-1.334810	1.468799
6	-4.068657	0.606162	0.744758
6	-4.001463	-0.956166	0.750695
1	-3.969748	1.039160	1.745887
1	-3.868275	-1.371708	1.755310
1	-5.016586	0.961714	0.324766
1	-4.914404	-1.395045	0.331937
6	-2.877557	1.001219	-0.193599
6	-2.779369	-1.254958	-0.182861
1	-2.927939	2.022650	-0.575618
1	-2.739563	-2.280400	-0.555570
6	-2.954037	-0.136976	-1.229253
1	-3.927635	-0.181269	-1.731801
1	-2.151979	-0.104952	-1.965987

Structure 5-6TS - NOR

B3LYP/GBS(1) = -1430.610710 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1430.909735 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1429.692046 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1431.006252 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1431.035937 a.u.
Enthalpy Correction = 0.422183
Gibbs Free Energy Correction = 0.349965

Atomic No	x-coord	y-coord	z-coord
7	1.550889	0.968006	1.230230
6	1.391916	2.274961	1.586176
6	0.469121	3.083751	1.006022
1	2.064080	2.651085	2.361235
1	0.349541	4.116604	1.319517
6	2.634518	0.275865	1.674358
6	3.002687	-0.934436	1.168052
1	3.222532	0.752856	2.462509
1	3.868972	-1.466995	1.547813
15	-0.548448	2.339775	-0.269318
15	2.011194	-1.513486	-0.198168
6	-0.275292	3.305127	-1.827894
1	-0.921722	2.916146	-2.622395
1	-0.492357	4.369422	-1.679430
1	0.764491	3.179534	-2.136405
6	-2.244251	2.970013	0.176199
1	-2.172068	4.046894	0.368866
1	-2.965546	2.812947	-0.631566
1	-2.607884	2.475168	1.080192
6	3.110254	-1.680835	-1.676705
1	3.946537	-2.360192	-1.474393
1	2.535784	-2.062256	-2.527734
1	3.494252	-0.691206	-1.933751
6	1.637446	-3.298880	0.143884
1	1.186345	-3.778930	-0.731601
1	2.564335	-3.830359	0.387221
1	0.950256	-3.386915	0.989475
77	0.349253	0.131924	-0.287773
1	1.347932	0.832289	-1.397900
1	-0.643279	-0.636644	-1.493219
6	-1.258988	-1.551896	-0.583413
6	-1.140648	-1.125084	0.815783
6	-2.749351	-1.455320	-0.929132
1	-2.991699	-1.452047	-1.995791
6	-2.576547	-0.749041	1.218254
1	-2.667863	-0.088696	2.085102
6	-3.409118	-2.612701	-0.117003
6	-3.345117	-2.097552	1.360036
6	-3.182378	-0.235721	-0.106558
1	-4.271052	-0.112078	-0.066260
1	-2.728952	0.679896	-0.472151
1	-4.444059	-2.754543	-0.447740
1	-2.890553	-3.567835	-0.258883
1	-4.353262	-1.938775	1.763392

1	-2.830333	-2.796154	2.028273
1	-0.762514	-2.458236	-0.923050
1	-0.627304	-1.789012	1.509502

Structure 6 - NOR

B3LYP/GBS(1) = -1430.611886 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1430.909723 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1429.695602 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1431.004686 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1431.033950 a.u.
Enthalpy Correction = 0.424717
Gibbs Free Energy Correction = 0.351895

Atomic No	x-coord	y-coord	z-coord
7	1.602006	0.960252	1.173215
6	1.481164	2.277187	1.515254
6	0.558772	3.097437	0.954762
1	2.185834	2.642607	2.264740
1	0.470275	4.136509	1.257041
6	2.683384	0.254512	1.609255
6	3.017485	-0.972995	1.126451
1	3.293174	0.742252	2.372519
1	3.882547	-1.511818	1.499555
15	-0.517047	2.346420	-0.264864
15	1.973320	-1.564980	-0.192603
6	-0.316424	3.296518	-1.843006
1	-1.001801	2.904310	-2.602652
1	-0.523865	4.362550	-1.693041
1	0.707162	3.164227	-2.199009
6	-2.191683	2.975125	0.256344
1	-2.107931	4.047227	0.469810
1	-2.943506	2.838364	-0.526676
1	-2.523137	2.460318	1.161399
6	3.024237	-1.807288	-1.695815
1	3.847085	-2.503799	-1.496612
1	2.416196	-2.198747	-2.518690
1	3.426143	-0.836462	-1.993596
6	1.559923	-3.327022	0.215372
1	1.059118	-3.817093	-0.626650
1	2.479692	-3.879769	0.437505
1	0.904907	-3.367698	1.089228
77	0.366173	0.137073	-0.274340
1	1.345704	0.793795	-1.450606
1	-0.789986	-0.759426	-1.462268
6	-1.318159	-1.536467	-0.664681
6	-1.136071	-1.080744	0.764876
6	-2.834978	-1.447151	-0.923093
1	-3.130497	-1.468481	-1.976681
6	-2.562445	-0.681707	1.194922
1	-2.617651	0.003827	2.045610
6	-3.470146	-2.569566	-0.053123
6	-3.349938	-2.007631	1.403114
6	-3.207642	-0.193383	-0.121786
1	-4.290730	-0.039487	-0.044980
1	-2.749221	0.701805	-0.534319

1	-4.517119	-2.718553	-0.340214
1	-2.960092	-3.531200	-0.182426
1	-4.342775	-1.817563	1.830982
1	-2.827762	-2.694262	2.078186
1	-0.874729	-2.491165	-0.951338
1	-0.695391	-1.821208	1.433820

Structure 4-7TS - NOR

B3LYP/GBS(1) = -1430.615208 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1430.914656 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1429.694528 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1431.012351 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1431.042086 a.u.
Enthalpy Correction = 0.421885
Gibbs Free Energy Correction = 0.349417

Atomic No	x-coord	y-coord	z-coord
7	2.222183	0.945989	-0.432256
6	3.314028	0.148293	-0.551431
6	3.269651	-1.204607	-0.384504
1	4.260130	0.647013	-0.780048
1	4.158220	-1.818150	-0.494236
6	2.363710	2.299332	-0.412414
6	1.326588	3.135047	-0.149080
1	3.364917	2.691508	-0.610783
1	1.449813	4.213783	-0.165722
15	1.681258	-1.862237	0.087618
15	-0.265906	2.356717	0.124258
6	1.890712	-2.762462	1.690911
1	0.939254	-3.208578	2.000807
1	2.642708	-3.555568	1.606362
1	2.201844	-2.043969	2.452782
6	1.312749	-3.272265	-1.058545
1	2.125123	-4.007249	-1.031212
1	0.382101	-3.774646	-0.772380
1	1.214786	-2.892451	-2.079249
6	-0.951802	3.090370	1.679076
1	-0.983859	4.184476	1.621884
1	-1.962902	2.713978	1.865622
1	-0.310367	2.788561	2.510659
6	-1.321232	3.169061	-1.177701
1	-2.388754	2.972009	-1.047389
1	-1.160862	4.253087	-1.151059
1	-1.009104	2.792833	-2.155932
77	0.332034	0.053994	0.081830
1	0.833977	0.291288	1.628088
1	-0.265366	-0.144195	-1.536799
6	-1.410017	-1.105268	-0.859481
6	-1.390661	-1.155924	0.601662
6	-2.787943	-0.550453	-1.228185
1	-2.884152	-0.119733	-2.228087
6	-2.789515	-0.695078	1.035099

1	-2.881986	-0.383134	2.078654
6	-3.743960	-1.754601	-0.946929
6	-3.751827	-1.848638	0.617231
6	-3.145029	0.351775	-0.030737
1	-4.204360	0.634866	-0.024257
1	-2.538939	1.247349	0.039245
1	-4.743616	-1.536223	-1.339157
1	-3.401897	-2.677823	-1.427938
1	-4.759453	-1.684350	1.017713
1	-3.410163	-2.823708	0.981616
1	-1.072659	-1.952196	-1.450519
1	-1.059341	-2.072934	1.088199

Structure 6-7TS - NOR

B3LYP/GBS(1) = -1430.6072678 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1430.903664 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1429.689162 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.995607 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1431.0260843 a.u.
Enthalpy Correction = 0.424766
Gibbs Free Energy Correction = 0.352273

Atomic No	x-coord	y-coord	z-coord
7	-2.084144	0.894902	-0.671391
6	-2.187116	2.244339	-0.866693
6	-1.204478	3.111146	-0.521582
1	-3.117086	2.583720	-1.324118
1	-1.299829	4.176151	-0.708285
6	-3.140356	0.083988	-0.972559
6	-3.155969	-1.249957	-0.711378
1	-3.989302	0.578854	-1.445931
1	-4.009222	-1.866014	-0.975841
15	0.275168	2.359020	0.150782
15	-1.682837	-1.871212	0.080204
6	0.631036	3.173815	1.776681
1	1.587875	2.819446	2.176432
1	0.676949	4.263779	1.670611
1	-0.162342	2.908087	2.479264
6	1.622197	3.085377	-0.904069
1	1.511541	4.175904	-0.929220
1	2.618062	2.842560	-0.525617
1	1.526830	2.697712	-1.921555
6	-2.172445	-2.663987	1.680234
1	-2.924619	-3.445233	1.521464
1	-1.296498	-3.111313	2.163281
1	-2.579668	-1.893071	2.338481
6	-1.143029	-3.351969	-0.895976
1	-0.260613	-3.817016	-0.443436
1	-1.948505	-4.094066	-0.935936
1	-0.892925	-3.042318	-1.913867
77	-0.422571	0.102548	0.208867
1	-1.317938	0.529643	1.538720
1	1.067270	-0.807630	1.601631
6	1.599948	-1.394021	0.791901
6	1.281278	-0.881155	-0.666007

6	3.115786	-1.134246	0.944315
1	3.476891	-1.181938	1.976990
6	2.635500	-0.264653	-1.096111
1	2.564243	0.478849	-1.894077
6	3.856547	-2.084552	-0.031763
6	3.597158	-1.435428	-1.431939
6	3.258970	0.221430	0.233130
1	4.301597	0.547748	0.131611
1	2.692879	1.009796	0.736270
1	4.926627	-2.116441	0.203811
1	3.482244	-3.112829	0.035748
1	4.533875	-1.067029	-1.871058
1	3.154961	-2.136838	-2.147908
1	1.311786	-2.436573	0.962557
1	1.036727	-1.722309	-1.316942

Structure 7 - NOR

B3LYP/GBS(1) = -1430.642393 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1430.935082 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1429.712647 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1431.019897 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1431.053084 a.u.
Enthalpy Correction = 0.425971
Gibbs Free Energy Correction = 0.350496

Atomic No	x-coord	y-coord	z-coord
7	0.525999	3.353907	0.339844
6	0.456835	3.978323	1.545539
6	0.687999	3.324287	2.720525
1	0.204031	5.043572	1.544841
1	0.634473	3.844003	3.672646
6	0.253698	4.005328	-0.820890
6	0.256296	3.376780	-2.033343
1	0.025085	5.073948	-0.753448
1	0.033720	3.920811	-2.946546
15	1.111078	1.583671	2.594927
15	0.607552	1.617860	-2.019512
6	-0.024715	0.671441	3.735311
1	0.232256	-0.391961	3.755410
1	0.037479	1.075724	4.752156
1	-1.050325	0.777639	3.372022
6	2.741236	1.408563	3.465970
1	2.679501	1.817968	4.480938
1	3.042230	0.358025	3.525354
1	3.505037	1.962046	2.911623
6	-0.784994	0.809387	-2.932148
1	-0.927824	1.287278	-3.908078
1	-0.581274	-0.254678	-3.081373
1	-1.703512	0.914426	-2.348303
6	2.022589	1.338586	-3.185388

1	2.224453	0.266373	-3.279002
1	1.801231	1.748423	-4.177463
1	2.917617	1.831180	-2.793924
77	0.975130	1.220468	0.275536
1	-0.540287	0.936435	0.462497
1	-0.175084	-1.336679	-1.069469
6	0.828732	-1.726754	-0.870980
6	1.627296	-0.774843	0.098331
6	0.710061	-3.054979	-0.093310
1	-0.066828	-3.725189	-0.477200
6	1.802402	-1.695053	1.344885
1	2.023004	-1.163686	2.273695
6	2.107527	-3.709786	0.005794
6	2.854278	-2.789009	1.024468
6	0.503286	-2.527365	1.343707
1	0.490221	-3.322272	2.100786
1	-0.400111	-1.915549	1.449380
1	2.034470	-4.738127	0.379817
1	2.606743	-3.755522	-0.969268
1	3.127805	-3.346880	1.929775
1	3.777686	-2.363534	0.614536
1	1.325423	-1.862046	-1.842269
1	2.639361	-0.607046	-0.331938

Structure 7-8TS - NOR

B3LYP/GBS(1) = -1430.621019 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1430.913484 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1429.675322 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1430.999385 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1431.034216 a.u.
Enthalpy Correction = 0.426037
Gibbs Free Energy Correction = 0.352097

Atomic No	x-coord	y-coord	z-coord
7	2.112182	0.934645	-0.711859
6	3.214730	0.156739	-0.953586
6	3.265235	-1.166761	-0.644837
1	4.071616	0.661024	-1.407176
1	4.146416	-1.764860	-0.854428
6	2.183374	2.290443	-0.906295
6	1.181706	3.134537	-0.547887
1	3.104021	2.667016	-1.358825
1	1.254079	4.204330	-0.718173
15	1.777282	-1.801649	0.128820
15	-0.240904	2.336321	0.205224
6	2.264518	-2.484354	1.781736
1	1.397901	-2.948391	2.265681
1	3.059273	-3.233138	1.685189
1	2.615369	-1.662599	2.411035
6	1.354374	-3.362156	-0.783299
1	2.199750	-4.060067	-0.774148
1	0.490902	-3.852818	-0.321681

1	1.106616	-3.117970	-1.819997
6	-0.443547	3.087200	1.889161
1	-0.514802	4.179456	1.830828
1	-1.347741	2.697769	2.369560
1	0.419819	2.813647	2.500914
6	-1.705227	3.069686	-0.669783
1	-2.638624	2.742426	-0.201324
1	-1.659149	4.164373	-0.632068
1	-1.707368	2.752266	-1.715865
77	0.424955	0.094199	0.136602
1	-0.604265	-0.320092	1.343095
1	-2.951219	-0.994393	2.308770
6	-2.814827	-0.586457	1.299893
1	-2.810064	0.505620	1.391047
6	-1.493710	-1.131552	0.647112
1	-1.195104	-2.030205	1.198803
6	-3.927345	-1.060358	0.327097
1	-4.909456	-1.166409	0.798261
6	-2.007524	-1.641003	-0.734418
1	-1.282841	-2.269787	-1.253638
6	-2.571005	-0.495332	-1.606993
6	-3.919523	-0.129546	-0.905295
6	-3.312030	-2.342431	-0.272597
1	-3.898705	-2.749681	-1.105785
1	-3.144178	-3.139413	0.461715
1	-2.742072	-0.848379	-2.630723
1	-1.868150	0.338125	-1.656408
1	-4.776086	-0.343172	-1.556007
1	-3.983596	0.927471	-0.624724

Structure 8 - NOR

B3LYP/GBS(1) = -1430.638477 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1430.929444 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -1429.688699 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -1431.010353 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -1431.043675 a.u.
Enthalpy Correction = 0.429824
Gibbs Free Energy Correction = 0.352554

Atomic No	x-coord	y-coord	z-coord
7	-2.619189	0.207237	-0.095323
6	-3.196125	1.449731	-0.109953
6	-2.471051	2.598939	-0.056668
1	-4.286412	1.468574	-0.165233
1	-2.950674	3.572541	-0.067987
6	-3.415269	-0.907202	-0.131683
6	-2.913600	-2.170116	-0.100435
1	-4.490241	-0.724069	-0.186138
1	-3.563331	-3.039138	-0.129362
15	-0.701866	2.339880	0.039413
15	-1.126104	-2.244831	-0.005404
6	-0.112438	3.281694	1.527037

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 1     0.979155    3.231959    1.604306
 1    -0.412622    4.334759    1.470968
 1    -0.545141    2.832595    2.424901
 6     0.054382    3.343126   -1.328084
 1    -0.246769    4.395145   -1.259952
 1     1.147629    3.287363   -1.280966
 1    -0.274477    2.938802   -2.289263
 6    -0.727223   -3.305281    1.465822
 1    -1.233112   -4.275760    1.398936
 1     0.352365   -3.478017    1.533586
 1    -1.056846   -2.791166    2.372545
 6    -0.578179   -3.356312   -1.388339
 1     0.504064   -3.517925   -1.340131
 1    -1.081439   -4.328930   -1.333948
 1    -0.819684   -2.882932   -2.343842
77    -0.601365    0.020490    0.003553
 1     1.165336   -0.139172    0.656334
 1     2.276769   -2.153335    0.835200
 6     2.737518   -1.556034    0.040736
 6     1.975029   -0.208443   -0.161283
 6     4.154993   -1.094054    0.455894
 1     4.744584   -1.875053    0.945205
 6     3.040635    0.860730    0.187441
 1     2.620642    1.839435    0.432041
 6     4.849071   -0.461141   -0.774412
 6     4.081160    0.890430   -0.958882
 6     3.834688    0.154731    1.307947
 1     4.728864    0.708016    1.618487
 1     3.229620   -0.066588    2.195437
 1     5.912184   -0.286495   -0.573496
 1     4.787708   -1.106444   -1.657846
 1     4.755941    1.746599   -0.843440
 1     3.608249    0.979828   -1.943196
 1     2.748898   -2.168307   -0.867938
 1     1.576154   -0.081198   -1.172480
```

6. Computational Details

6.1. GBS2 Basis set

This basis set is LANL2TZ+(3f).
It was obtained in the same way as described in Yates, B.F. J. Mol. Struct. (Theochem), 2000, 506, 223-232 for platinum.
a) The triple-zeta split was obtained by uncontracting the LANL2DZ basis set of Hay and Wadt to give:
[341/321/21] -> [3311/3111/111]
b) The f-function exponent (0.9380) was taken from Frenking and co-workers (Chem. Phys. Lett., 1993, 208, 111-114) and then split according to the even scaling rule to give three exponents (3.752, 0.938, 0.2345).
c) Diffuse s, p and d functions were added using an even tempered extension of the two outermost exponents. This gave exponents of s=0.014304, p=0.008582 and d=0.05031.

```
-C -H -N -O -P -S 0
6-311+G(2d,p)
****
-Ir 0
 S   3 1.00       0.000000000000
      0.2350000000D+01 -0.1678464034D+01
      0.1582000000D+01  0.2095255043D+01
      0.5018000000D+00  0.4162934085D+00
 S   3 1.00       0.000000000000
      0.2350000000D+01  0.1646447056D+01
      0.1582000000D+01 -0.2274815077D+01
      0.5018000000D+00 -0.1049436036D+01
 S   1 1.00       0.000000000000
      0.2500000000D+00  0.1216779041D+01
 S   1 1.00       0.000000000000
      0.5980000000D-01  0.1000000000D+01
 S   1 1.00       0.000000000000
      0.1430400000D-01  0.1000000000D+01
 P   3 1.00       0.000000000000
      0.2792000000D+01 -0.3889211885D+00
      0.1541000000D+01  0.9077515732D+00
      0.5285000000D+00  0.4691442862D+00
 P   1 1.00       0.000000000000
      0.5100000000D+00 -0.1170669243D+00
 P   1 1.00       0.000000000000
      0.9800000000D-01  0.1048900218D+01
 P   1 1.00       0.000000000000
      0.2900000000D-01  0.1000000000D+01
 P   1 1.00       0.000000000000
      0.8582000000D-02  0.1000000000D+01
 D   1 1.00       0.000000000000
      0.1240000000D+01  0.5087021868D+00
 D   1 1.00       0.000000000000
      0.4647000000D+00  0.5862101848D+00
 D   1 1.00       0.000000000000
      0.1529000000D+00  0.1000000000D+01
 D   1 1.00       0.000000000000
      0.5031000000D-01  0.1000000000D+01
 F   1 1.00       0.000000000000
      3.7520000000D+00  0.1000000000D+01
 F   1 1.00       0.000000000000
      0.9380000000D+00  0.1000000000D+01
 F   1 1.00       0.000000000000
      0.2345000000D+00  0.1000000000D+01
 ****

Ir 0
lanl2dz
```

6.2. Theoretical Models and Structural Comparisons

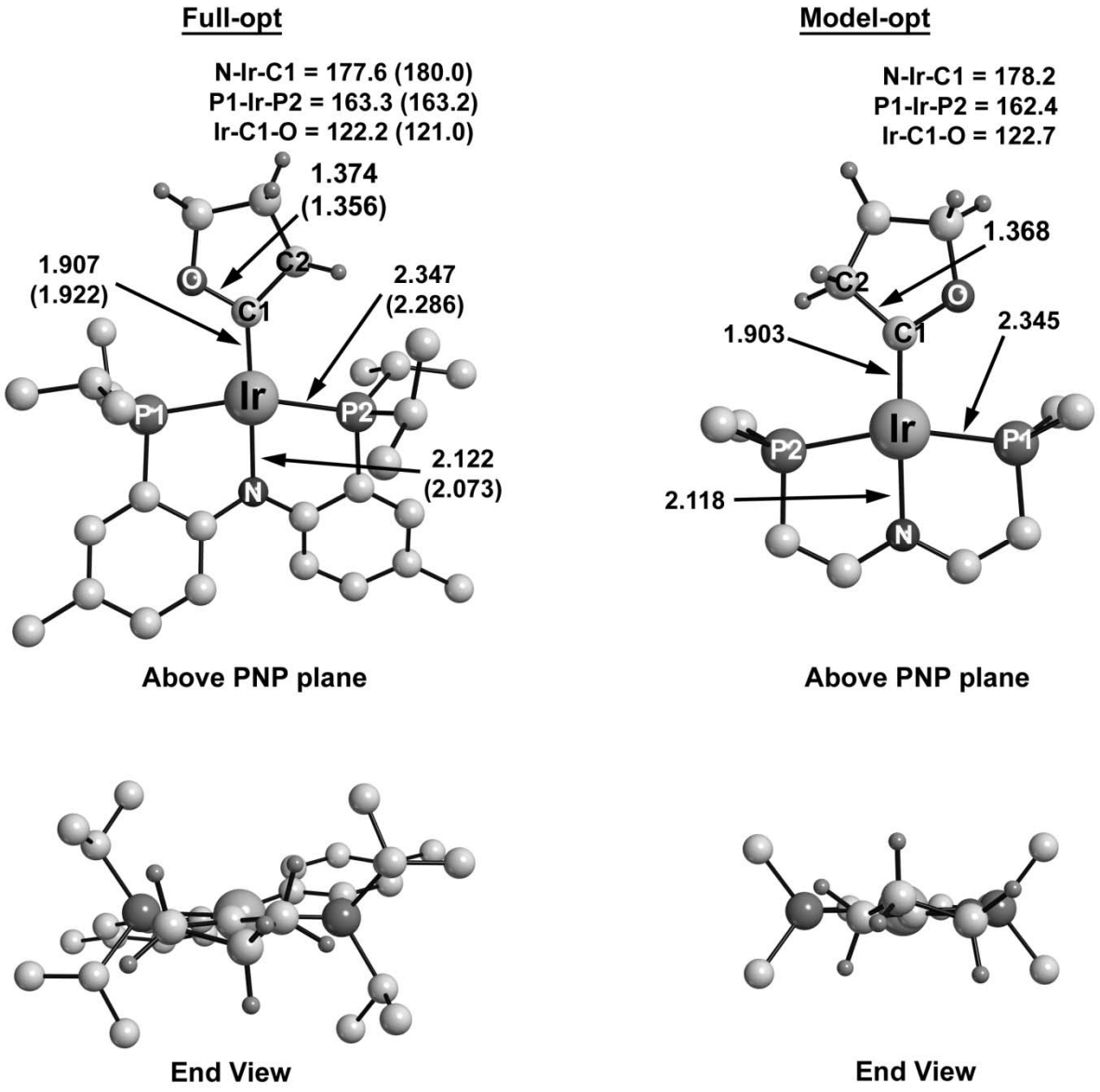

Figure S26. Diagram displaying the Model-opt, Full-opt computational models used. The Model-opt has replaced the isopropyl groups with methyl groups and the aromatic rings with ethylene bridges. Parameters displayed and Full-opt, Model-opt and experimental[2] (in parentheses) bond lengths and angles in the experimentally obtained $\mathbf{8}_{\mathbf{THF}}$. All figures in Angstroms.

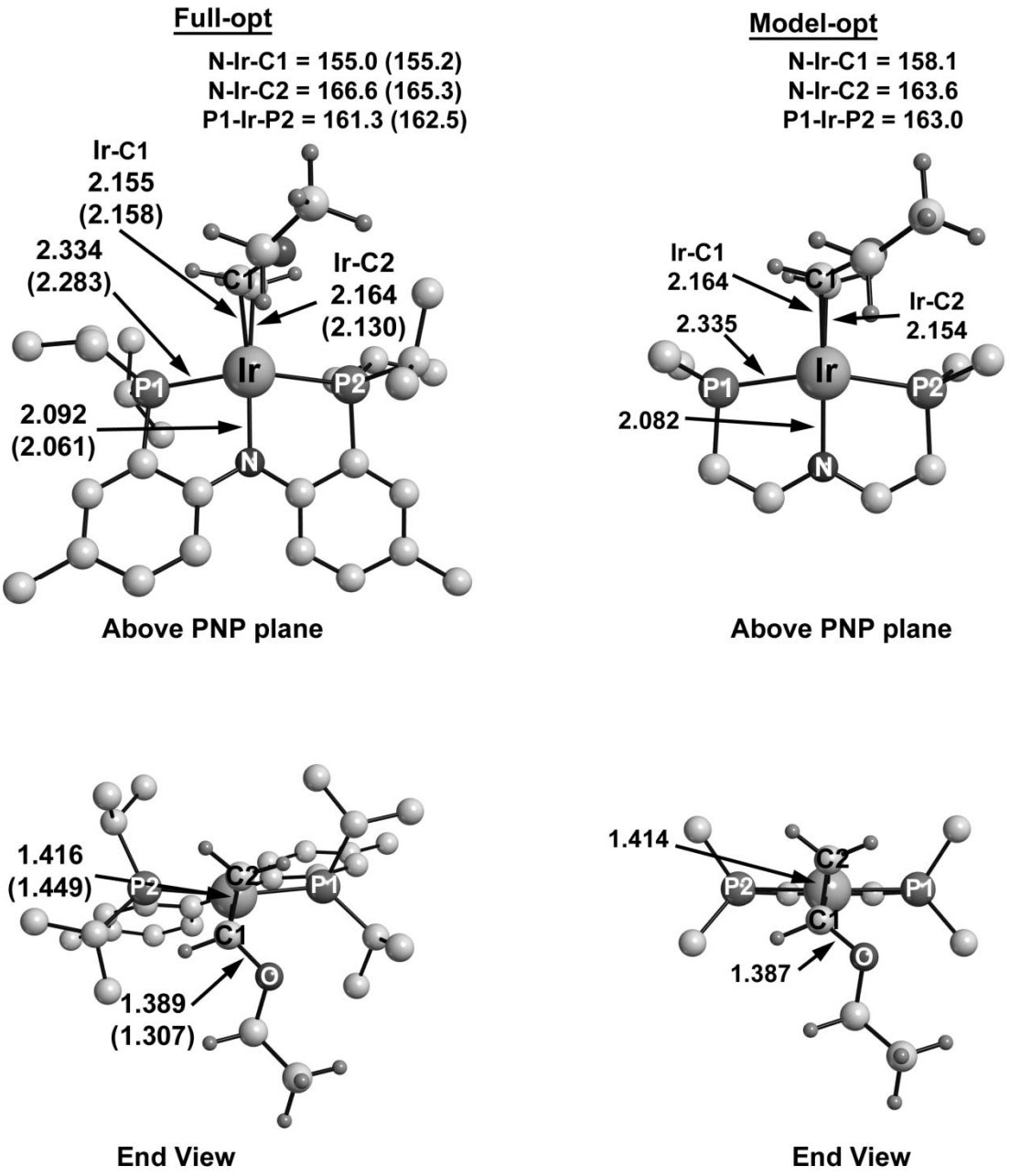

Figure S27. Diagram displaying the Model-opt, Full-opt computational models used. The Model-opt has replaced the isopropyl groups with methyl groups and the aromatic rings with ethylene bridges. Parameters displayed and Full-opt, Model-opt and experimental[2] (in parentheses) bond lengths and angles in the experimentally obtained $\mathbf{16}_{\mathbf{DEE}}$. All figures in Angstroms.

6.3. Rationale for the use of MP2/GBS2

B3LYP does not account for dispersive interactions and hence the absolute value of the transition barriers and reaction endpoints, when considering large full ligand models of organometallic

complexes, are prone to uncertainty. However the relative energies are still justifiable provided the steric environment does not change significantly throughout the reaction relative energy surface. But in situations where steric environment does significantly change, care must be taken when interpreting the calculations. A rare example of this "significant" change occurs in the reaction involving formation of the free vinyl ether.

Take the formation of **1** + $\mathbf{11_{THF}}$ in Figure 8. Its energy is calculated as follows:
THF + C_7H_{10} → $\mathbf{11_{THF}}$ + C_7H_{12} ; $\Delta E=(E_{11THF} + E_{C7H12})-(E_{THF} + E_{C7H10})$
This reaction energy (ΔE) is completely <u>independent</u> of the (PNP)Ir precursor, the level of theory and dispersive environment surrounding the (PNP)Ir structure.

But now consider a different coordinate on the same relative energy surface. Take $\mathbf{5}_{THF}$.
1 + C_7H_{10} + THF → $\mathbf{5_{THF}}$ + C_7H_{12} ; $\Delta E=(E_{\mathbf{5THF}} + E_{C7H12}) – (E_{\mathbf{1}} + E_{C7H10} + E_{THF})$
This reaction energy is <u>dependent</u> on the structure, the level of theory and the dispersive environment present for the (PNP)Ir structure. In fact every coordinate on the surface (except structure 11_{THF}) has this same dependency and hence comparison is possible.

But in order to compare the dependent and independent cases outlined ($\mathbf{11_{THF}}$ and $\mathbf{5_{THF}}$ in the example above), the level of theory must be chosen carefully. Ideally a functional that combines dispersive interactions with sound thermochemical modelling would be used, but unfortunately this is currently unavailable for third row transition metals. An alternative is to use perturbation theory which in itself has limitations,[7] but is capable of reducing the error between the independent and dependent cases above.

The main aim for our use of MP2 within this manuscript is not to introduce another level of theory but to attempt to rectify (or improve the accuracy of) a clear error in one coordinate on our relative energy surfaces. It is not feasible to use it to provide an alternative level of theory due to computational limitations.

6.4. B3LYP vs M06 Full-opt level of theory comparison diagram

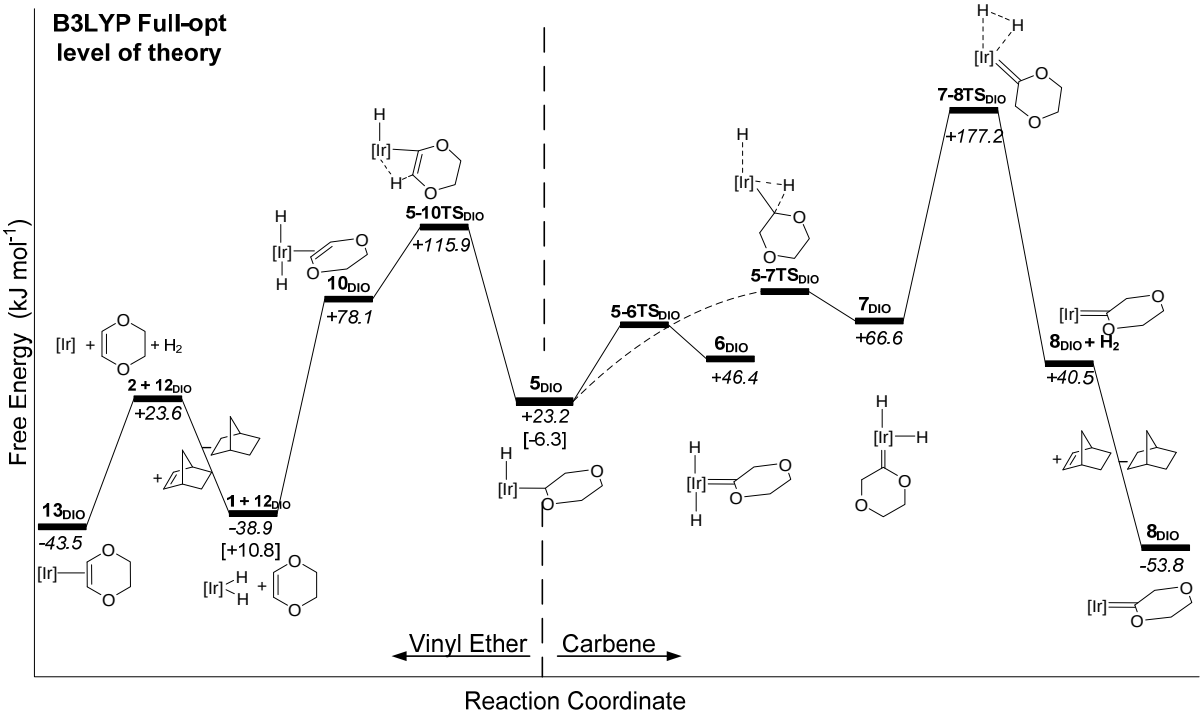

Figure S28. Full-opt comparison diagram for the Dioxane + IrH_2 reaction. Values in italics are B3LYP gibbs corrected energies using the full ligand molecule. Those in square brackets are MP2 gibbs corrected energies using the full ligand molecule.

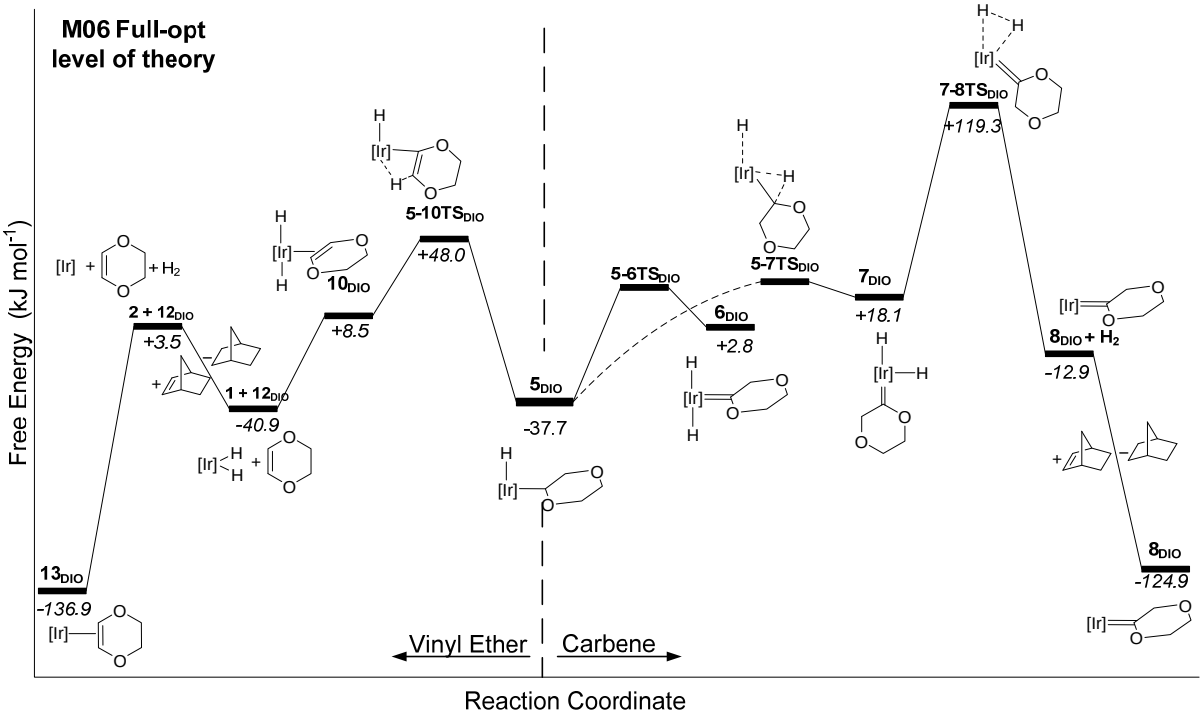

Figure S29. Full-opt comparison diagram for the Dioxane + IrH_2 reaction. Values in italics are M06 gibbs corrected energies using the full ligand molecule.

7. References

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